



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2020 – 03:01 AM EDT

PDB ID : 6O3M
Title : Unmodified tRNA(Pro) bound to Thermus thermophilus 70S (cognate)
Authors : Hoffer, E.D.; Subaramanian, S.; Hong, S.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-02-26
Resolution : 3.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

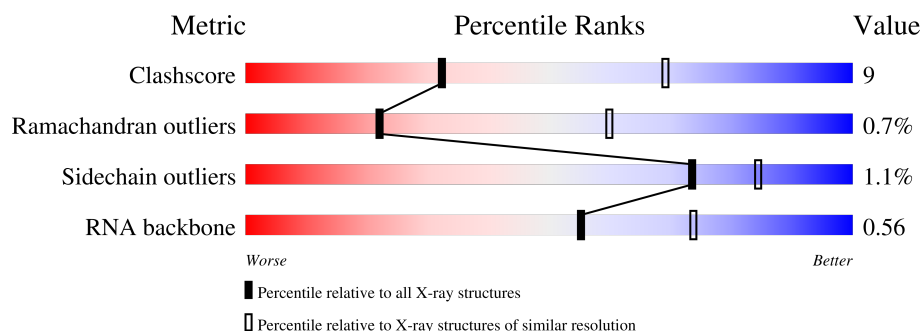
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 141614 | 1099 (4.26-3.70) |
| Ramachandran outliers | 138981 | 1061 (4.26-3.70) |
| Sidechain outliers | 138945 | 1053 (4.26-3.70) |
| RNA backbone | 3102 | 1041 (4.84-3.00) |













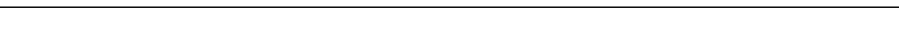

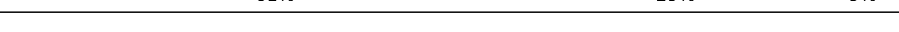

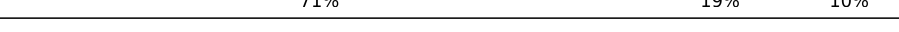








The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS failed to run properly.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | QA | 1521 | |
| 1 | XA | 1521 | |
| 2 | QB | 256 | |
| 2 | XB | 256 | |
| 3 | QC | 239 | |
| 3 | XC | 239 | |














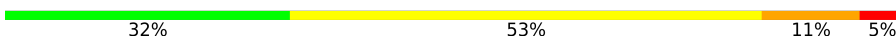











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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 4 | QD | 209 |  |
| 4 | XD | 209 |  |
| 5 | QE | 162 |  |
| 5 | XE | 162 |  |
| 6 | QF | 101 |  |
| 6 | XF | 101 |  |
| 7 | QG | 156 |  |
| 7 | XG | 156 |  |
| 8 | QH | 138 |  |
| 8 | XH | 138 |  |
| 9 | QI | 128 |  |
| 9 | XI | 128 |  |
| 10 | QJ | 105 |  |
| 10 | XJ | 105 |  |
| 11 | QK | 129 |  |
| 11 | XK | 129 |  |
| 12 | QL | 132 |  |
| 12 | XL | 132 |  |
| 13 | QM | 126 |  |
| 13 | XM | 126 |  |
| 14 | QN | 61 |  |
| 14 | XN | 61 |  |
| 15 | QO | 89 |  |
| 15 | XO | 89 |  |
| 16 | QP | 88 |  |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 16 | XP | 88 |  |
| 17 | QQ | 105 |  |
| 17 | XQ | 105 |  |
| 18 | QR | 88 |  |
| 18 | XR | 88 |  |
| 19 | QS | 93 |  |
| 19 | XS | 93 |  |
| 20 | QT | 106 |  |
| 20 | XT | 106 |  |
| 21 | QU | 27 |  |
| 21 | XU | 27 |  |
| 22 | QV | 77 |  |
| 22 | XV | 77 |  |
| 23 | QX | 19 |  |
| 23 | XX | 19 |  |
| 24 | RA | 2915 |  |
| 24 | YA | 2915 |  |
| 25 | RB | 122 |  |
| 25 | YB | 122 |  |
| 26 | RD | 276 |  |
| 26 | YD | 276 |  |
| 27 | RE | 206 |  |
| 27 | YE | 206 |  |
| 28 | RF | 210 |  |
| 28 | YF | 210 |  |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 29 | RG | 182 |  74% 24% ... |
| 29 | YG | 182 |  68% 29% .. |
| 30 | RH | 180 |  69% 26% .. |
| 30 | YH | 180 |  78% 17% .. |
| 31 | RI | 148 |  82% 16% .. |
| 31 | YI | 148 |  85% 12% .. |
| 32 | RN | 140 |  80% 19% . |
| 32 | YN | 140 |  80% 18% .. |
| 33 | RO | 122 |  74% 26% |
| 33 | YO | 122 |  80% 20% |
| 34 | RP | 150 |  70% 30% |
| 34 | YP | 150 |  75% 23% . |
| 35 | RQ | 141 |  73% 26% . |
| 35 | YQ | 141 |  72% 26% . |
| 36 | RR | 118 |  75% 24% .. |
| 36 | YR | 118 |  84% 15% . |
| 37 | RS | 112 |  71% 29% . |
| 37 | YS | 112 |  76% 23% . |
| 38 | RT | 146 |  70% 22% . 6% |
| 38 | YT | 146 |  69% 23% . 6% |
| 39 | RU | 118 |  85% 13% .. |
| 39 | YU | 118 |  81% 17% .. |
| 40 | RV | 101 |  74% 24% . |
| 40 | YV | 101 |  74% 25% . |
| 41 | RW | 113 |  79% 21% |



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 41 | YW | 113 |  85% 14% . |
| 42 | RX | 96 |  82% 14% . |
| 42 | YX | 96 |  81% 15% . |
| 43 | RY | 110 |  75% 22% . |
| 43 | YY | 110 |  70% 27% . |
| 44 | RZ | 206 |  67% 21% 11% |
| 44 | YZ | 206 |  69% 18% . 11% |
| 45 | R0 | 85 |  75% 20% 5% |
| 45 | Y0 | 85 |  65% 22% 13% |
| 46 | R1 | 98 |  81% 18% . |
| 46 | Y1 | 98 |  78% 17% 5% |
| 47 | R2 | 72 |  72% 24% . |
| 47 | Y2 | 72 |  74% 22% . |
| 48 | R3 | 60 |  83% 15% . |
| 48 | Y3 | 60 |  73% 20% 5% . |
| 49 | R4 | 71 |  72% 25% . |
| 49 | Y4 | 71 |  58% 37% . . |
| 50 | R5 | 60 |  72% 27% . |
| 50 | Y5 | 60 |  75% 22% . . |
| 51 | R6 | 54 |  80% 19% . |
| 51 | Y6 | 54 |  67% 31% . |
| 52 | R7 | 49 |  86% 10% . |
| 52 | Y7 | 49 |  82% 16% . |
| 53 | R8 | 65 |  68% 28% . . |
| 53 | Y8 | 65 |  72% 23% . . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 54 | R9 | 37 |  <div>70%30%</div> |
| 54 | Y9 | 37 |  <div>84%16%</div> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 56 | SF4 | XD | 301 | - | - | X | - |

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 291782 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | QA | 1500 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32247 | 14353 | 5981 | 10414 | 1499 | | | |
| 1 | XA | 1500 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32249 | 14354 | 5984 | 10412 | 1499 | | | |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | QB | 235 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1907 | 1217 | 342 | 343 | 5 | | | |
| 2 | XB | 236 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1915 | 1223 | 343 | 344 | 5 | | | |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | QC | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1011 | 313 | 280 | 1 | | | |
| 3 | XC | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1011 | 313 | 280 | 1 | | | |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | QD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1703 | 1066 | 339 | 291 | 7 | | | |
| 4 | XD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1703 | 1066 | 339 | 291 | 7 | | | |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | QE | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |
| 5 | XE | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | QF | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |
| 6 | XF | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | QG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |
| 7 | XG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | QH | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1108 | 700 | 214 | 192 | 2 | | | |
| 8 | XH | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1108 | 700 | 214 | 192 | 2 | | | |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9 | QI | 125 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 989 | 627 | 191 | 171 | | | | |
| 9 | XI | 126 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 998 | 633 | 193 | 172 | | | | |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | QJ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 801 | 504 | 157 | 139 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | XJ | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 777 | 487 | 153 | 136 | 1 | | | |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | QK | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 549 | 168 | 165 | 3 | | | |
| 11 | XK | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 864 | 537 | 164 | 160 | 3 | | | |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | QL | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 975 | 614 | 196 | 164 | 1 | | | |
| 12 | XL | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 956 | 603 | 193 | 159 | 1 | | | |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | QM | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 955 | 591 | 197 | 165 | 2 | | | |
| 13 | XM | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 946 | 585 | 195 | 164 | 2 | | | |

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14 | QN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |
| 14 | XN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | QO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |
| 15 | XO | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 729 | 457 | 146 | 124 | 2 | | | |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | QP | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 705 | 446 | 140 | 118 | 1 | | | |
| 16 | XP | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 705 | 446 | 140 | 118 | 1 | | | |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | QQ | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |
| 17 | XQ | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18 | QR | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 574 | 367 | 112 | 95 | | | |
| 18 | XR | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 574 | 367 | 112 | 95 | | | |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | QS | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 424 | 124 | 115 | 2 | | | |
| 19 | XS | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 674 | 430 | 126 | 116 | 2 | | | |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | QT | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 470 | 162 | 129 | 2 | | | |
| 20 | XT | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 470 | 162 | 129 | 2 | | | |

- Molecule 21 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | QU | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |
| 21 | XU | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |

- Molecule 22 is a RNA chain called P-site ASLPro.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22 | QV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1647 | 733 | 295 | 542 | 77 | | | |
| 22 | XV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1647 | 733 | 295 | 542 | 77 | | | |

- Molecule 23 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 23 | QX | 19 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 418 | 186 | 86 | 127 | 19 | | | |
| 23 | XX | 19 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 418 | 186 | 86 | 127 | 19 | | | |

- Molecule 24 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 24 | RA | 2882 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62071 | 27627 | 11611 | 19952 | 2881 | | | |
| 24 | YA | 2883 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62091 | 27636 | 11613 | 19960 | 2882 | | | |

- Molecule 25 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 25 | RB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |
| 25 | YB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 26 | RD | 272 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2115 | 1335 | 420 | 357 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 26 | YD | 272 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2115 | 1335 | 420 | 357 | 3 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | RE | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1568 | 991 | 300 | 271 | 6 | | | |
| 27 | YE | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1568 | 991 | 300 | 271 | 6 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 28 | RF | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1011 | 297 | 275 | 2 | | | |
| 28 | YF | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1011 | 297 | 275 | 2 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29 | RG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |
| 29 | YG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | RH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1336 | 848 | 251 | 236 | 1 | | | |
| 30 | YH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1336 | 848 | 251 | 236 | 1 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | RI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |
| 31 | YI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | RN | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |
| 32 | YN | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | RO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |
| 33 | YO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | RP | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1145 | 712 | 232 | 198 | 3 | | | |
| 34 | YP | 147 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 698 | 229 | 192 | 3 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | RQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |
| 35 | YQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 36 | RR | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | |
| 36 | YR | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 37 | RS | 111 | Total | C | N | O | 0 | 0 | 0 |
| | | | 882 | 556 | 176 | 150 | | | |
| 37 | YS | 111 | Total | C | N | O | 0 | 0 | 0 |
| | | | 882 | 556 | 176 | 150 | | | |

- Molecule 38 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | RT | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |
| 38 | YT | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |

- Molecule 39 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | RU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |
| 39 | YU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | RV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |
| 40 | YV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | RW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 900 | 566 | 177 | 155 | 2 | | | |
| 41 | YW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 900 | 566 | 177 | 155 | 2 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 42 | RX | 92 | Total | C | N | O | 0 | 0 | 0 |
| | | | 725 | 471 | 131 | 123 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 42 | YX | 92 | Total | C | N | O | 0 | 0 | 0 |
| | | | 725 | 471 | 131 | 123 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | RY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 818 | 525 | 155 | 132 | 6 | | | |
| 43 | YY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 818 | 525 | 155 | 132 | 6 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | RZ | 183 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1461 | 933 | 260 | 265 | 3 | | | |
| 44 | YZ | 183 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1461 | 933 | 260 | 265 | 3 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | R0 | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 643 | 398 | 137 | 107 | 1 | | | |
| 45 | Y0 | 74 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 593 | 367 | 126 | 99 | 1 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | R1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 481 | 150 | 131 | 1 | | | |
| 46 | Y1 | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 729 | 457 | 145 | 126 | 1 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | R2 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 358 | 118 | 104 | 1 | | | |
| 47 | Y2 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 358 | 118 | 104 | 1 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 48 | R3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |
| 48 | Y3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49 | R4 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 565 | 356 | 103 | 101 | 5 | | | |
| 49 | Y4 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 565 | 356 | 103 | 101 | 5 | | | |

- Molecule 50 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50 | R5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |
| 50 | Y5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51 | R6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 453 | 281 | 91 | 77 | 4 | | | |
| 51 | Y6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 453 | 281 | 91 | 77 | 4 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 52 | R7 | 47 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 409 | 251 | 102 | 54 | 2 | | | |
| 52 | Y7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |

- Molecule 53 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 53 | R8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |
| 53 | Y8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |

- Molecule 54 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 54 | R9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |
| 54 | Y9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

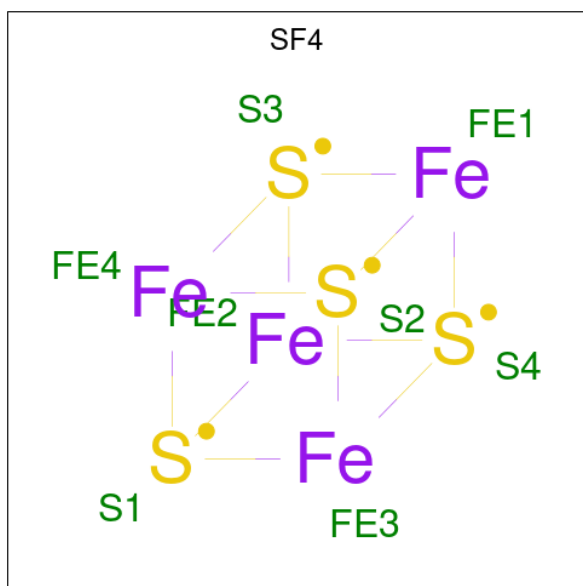
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 55 | QA | 69 | Total | Mg | 0 | 0 |
| | | | 69 | 69 | | |
| 55 | YA | 454 | Total | Mg | 0 | 0 |
| | | | 454 | 454 | | |
| 55 | Y5 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | YR | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 55 | XE | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | YD | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 55 | QV | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | XA | 67 | Total | Mg | 0 | 0 |
| | | | 67 | 67 | | |
| 55 | RQ | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | Y0 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | YQ | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 55 | RD | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | R1 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | Y7 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 55 | QH | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | RA | 381 | Total 381 | Mg 381 | 0 | 0 |
| 55 | YP | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | RE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | YB | 8 | Total 8 | Mg 8 | 0 | 0 |
| 55 | RB | 9 | Total 9 | Mg 9 | 0 | 0 |
| 55 | QE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | YE | 1 | Total 1 | Mg 1 | 0 | 0 |

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|--------|---------|---------|
| 56 | QD | 1 | Total 8 | Fe 4 | S 4 | 0 | 0 |
| 56 | XD | 1 | Total 8 | Fe 4 | S 4 | 0 | 0 |

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

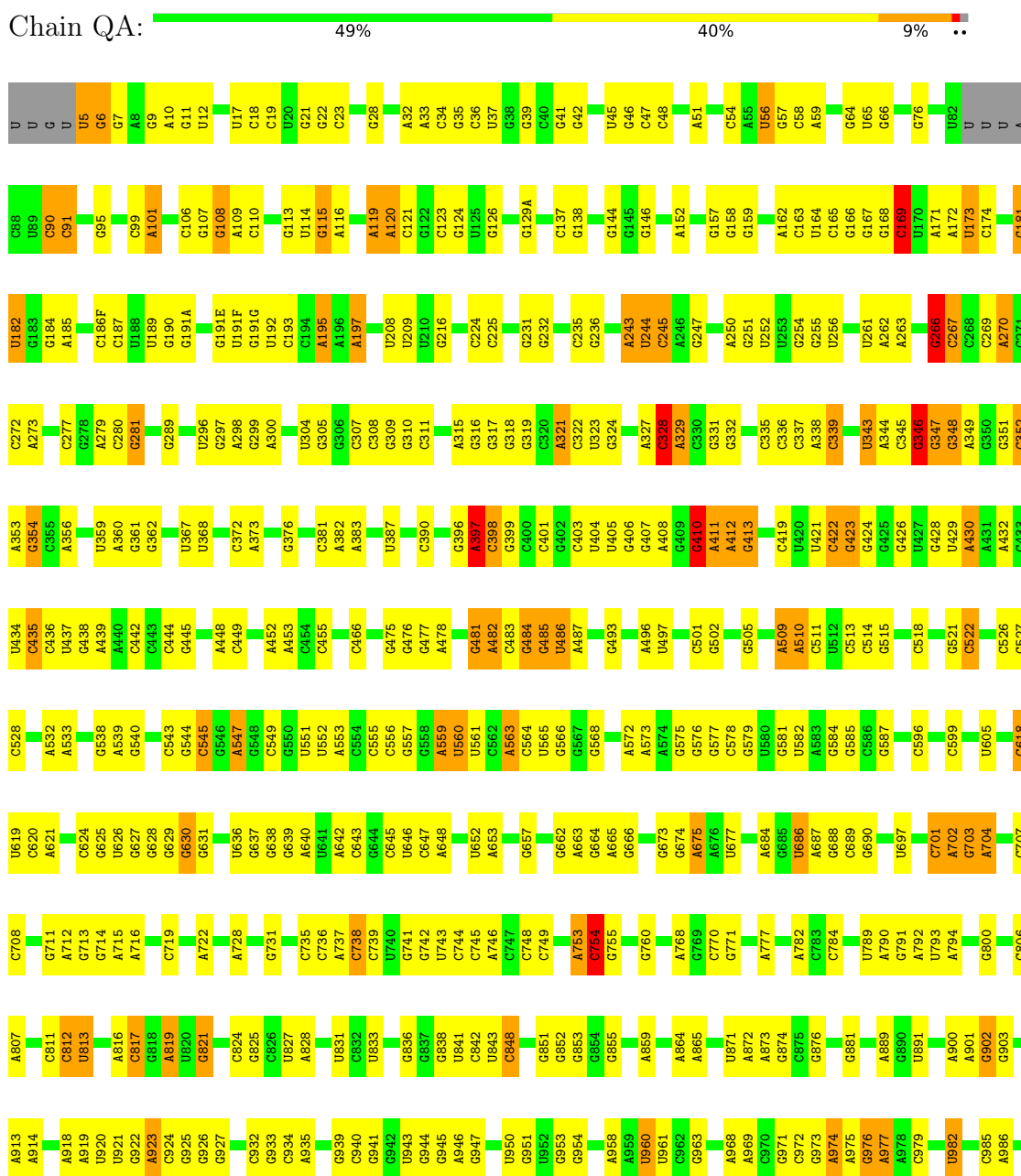
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 57 | Y9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | YY | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | Y6 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | QN | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | XN | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | RY | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | Y4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | R6 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | Y5 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | R5 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | R4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | R9 | 1 | Total 1 | Zn 1 | 0 | 0 |

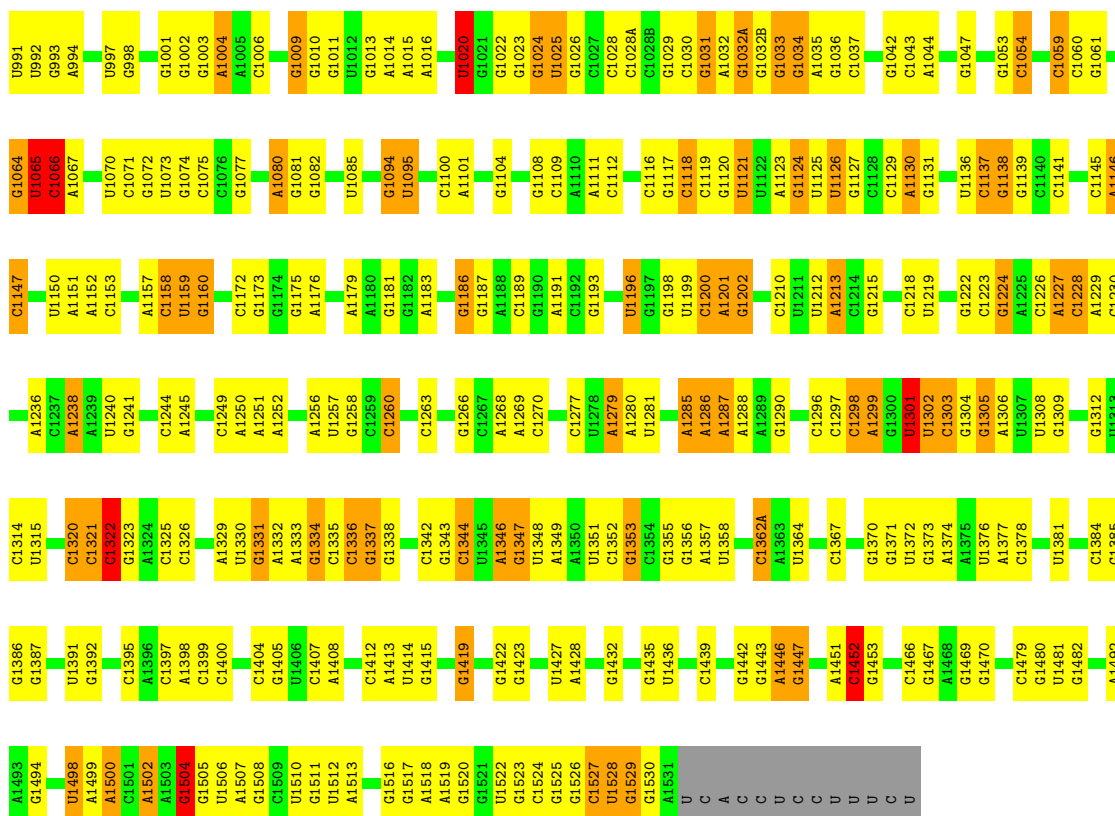
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

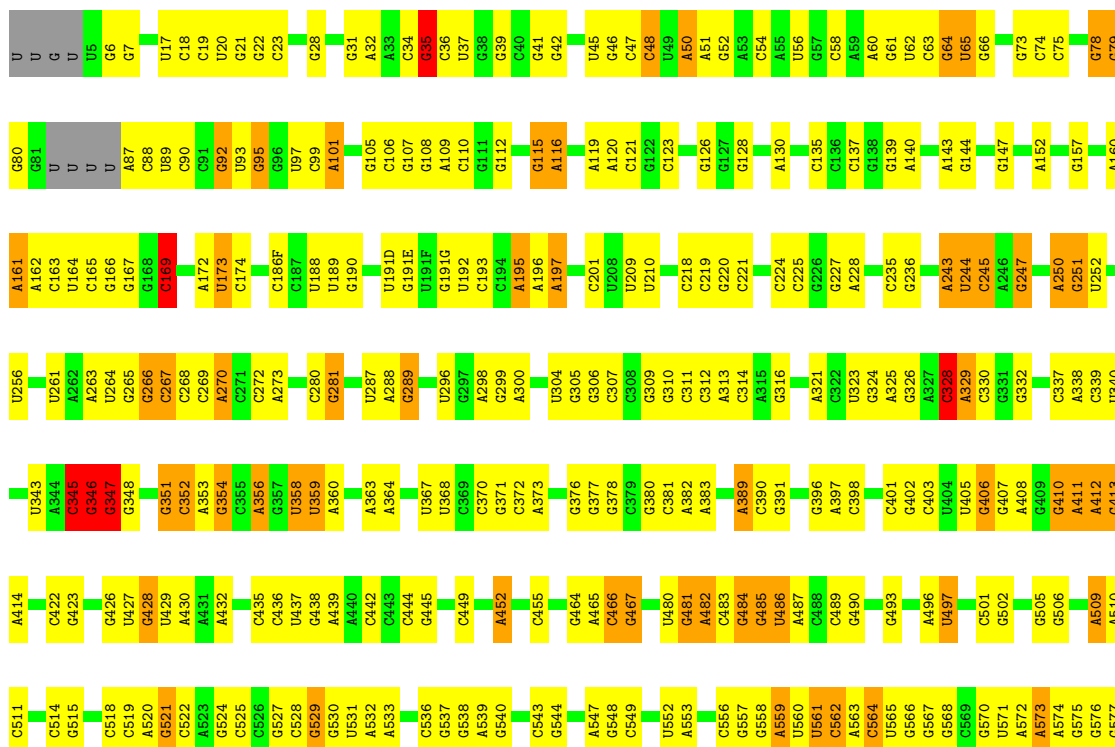
• Molecule 1: 16S rRNA

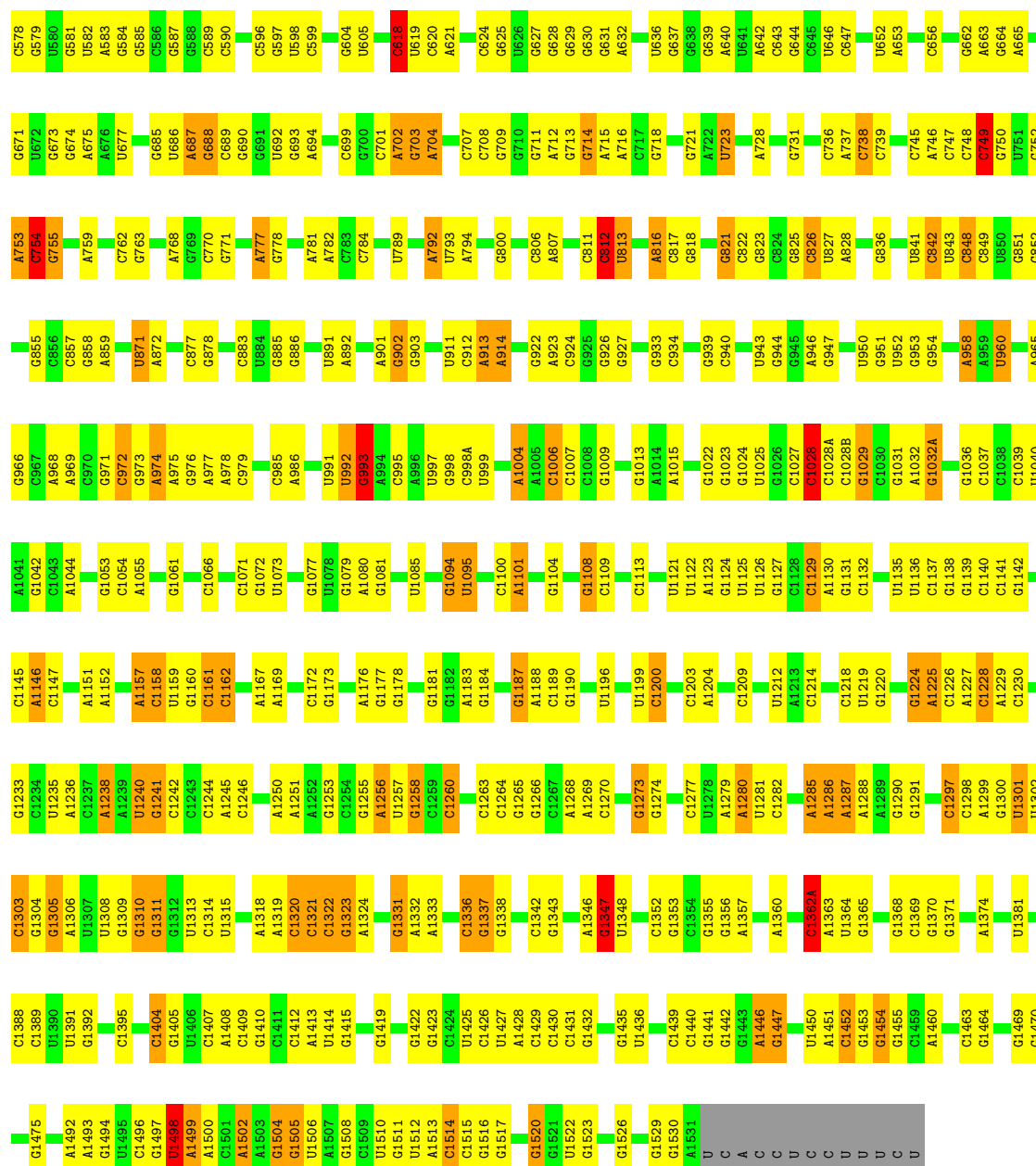




- Molecule 1: 16S rRNA

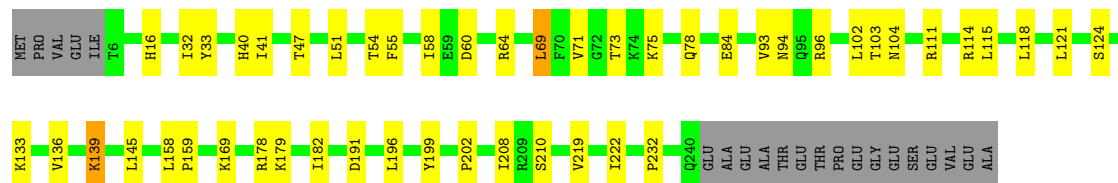
Chain XA:  48% 40% 9% 3%

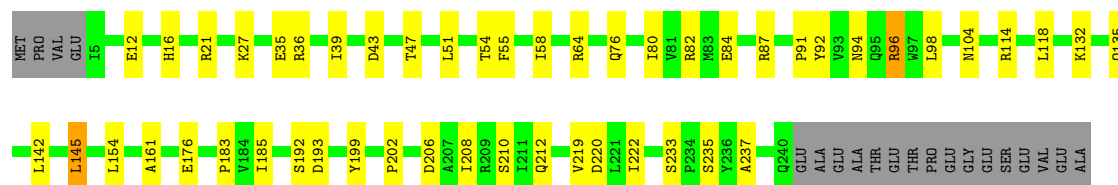




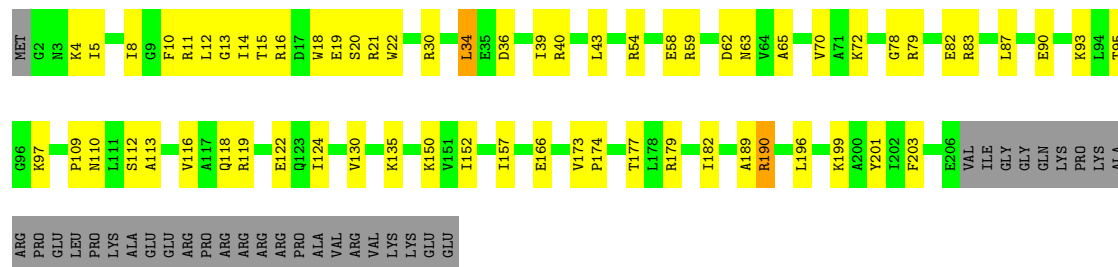
• Molecule 2: 30S ribosomal protein S2

Chain QB: 73% 18% 8%

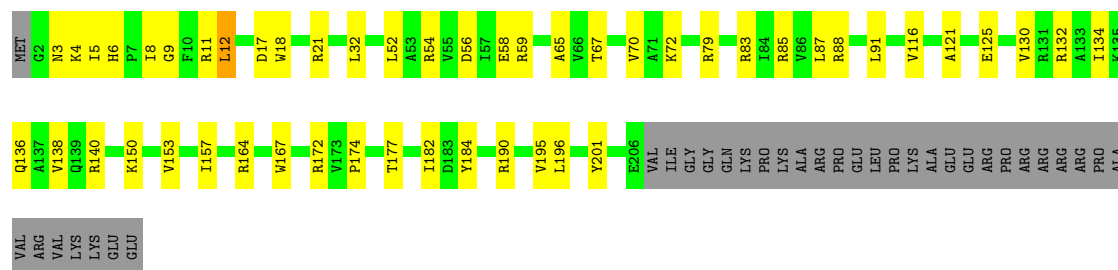




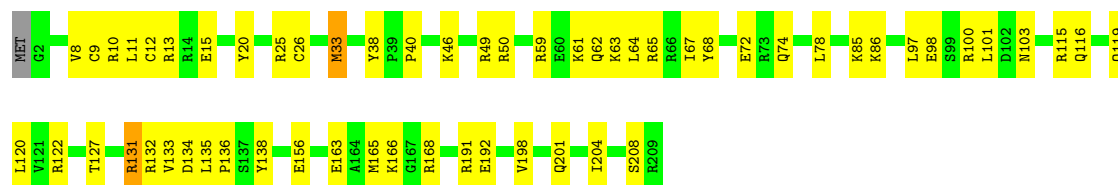
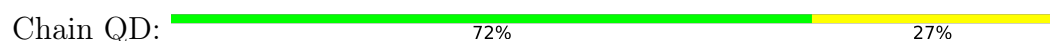
• Molecule 3: 30S ribosomal protein S3



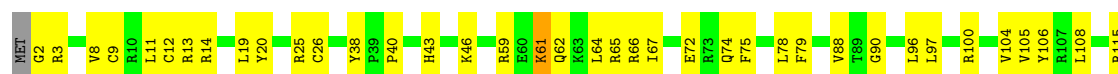
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4



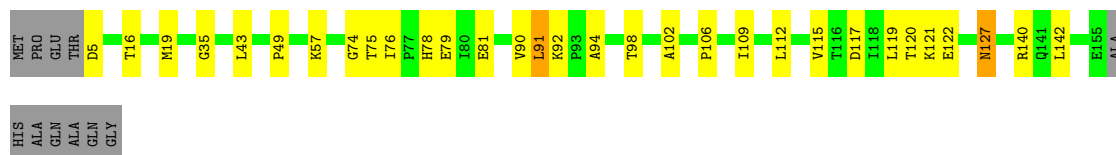
• Molecule 4: 30S ribosomal protein S4





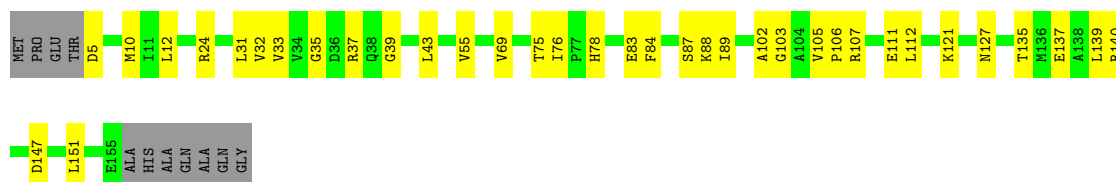
- Molecule 5: 30S ribosomal protein S5

Chain QE: 74% 18% 7%



- Molecule 5: 30S ribosomal protein S5

Chain XE: 71% 22% 7%



- Molecule 6: 30S ribosomal protein S6

Chain QF: 77% 23%



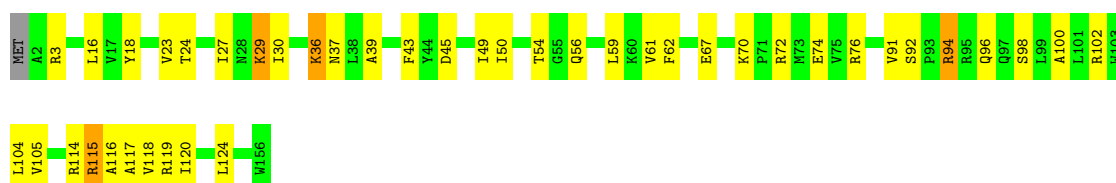
- Molecule 6: 30S ribosomal protein S6

Chain XF: 88% 12%




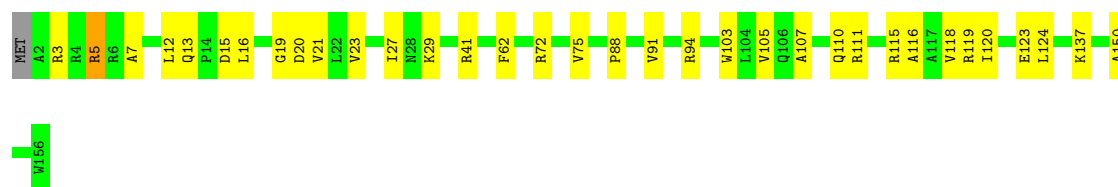
- Molecule 7: 30S ribosomal protein S7

Chain QG: 72% 24% 4%



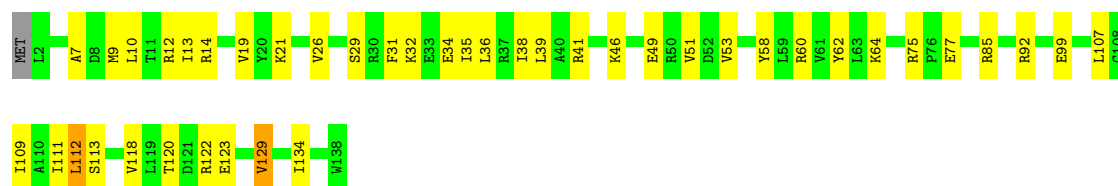
- Molecule 7: 30S ribosomal protein S7

Chain XG:  78% 21% ..



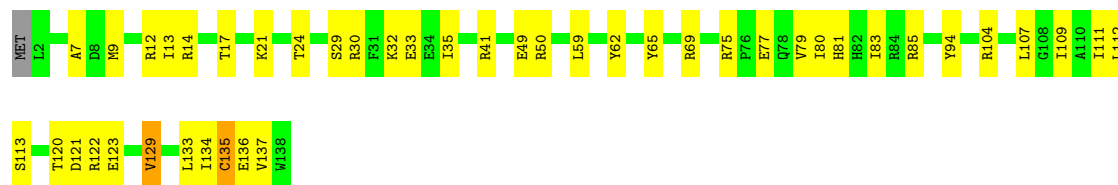
- Molecule 8: 30S ribosomal protein S8

Chain QH:  69% 29% ..



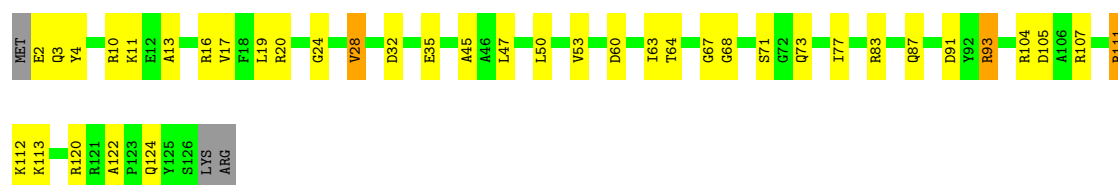
- Molecule 8: 30S ribosomal protein S8

Chain XH:  67% 30% ..



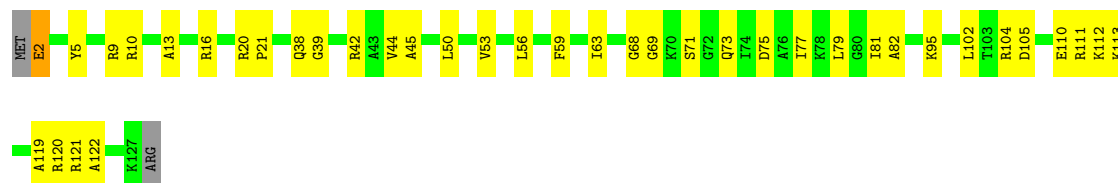
- Molecule 9: 30S ribosomal protein S9

Chain QI:  67% 28% ..

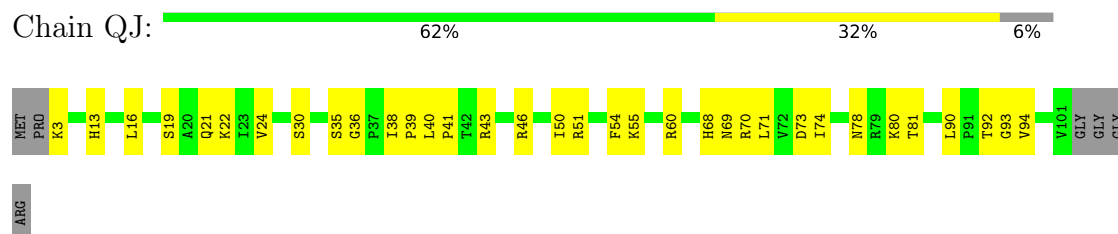


- Molecule 9: 30S ribosomal protein S9

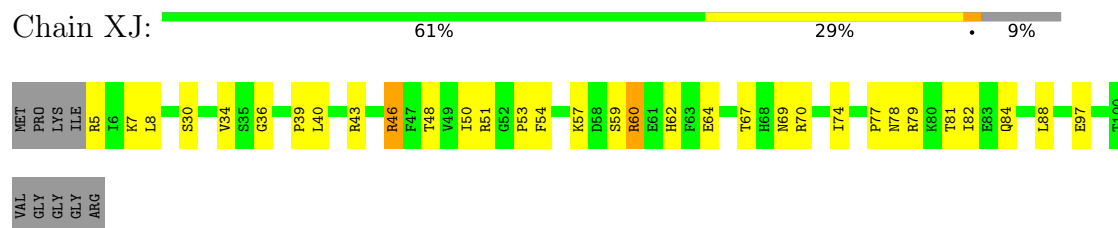
Chain XI:  68% 30% ..



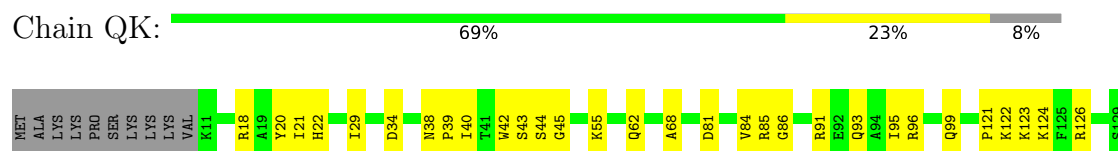
- Molecule 10: 30S ribosomal protein S10



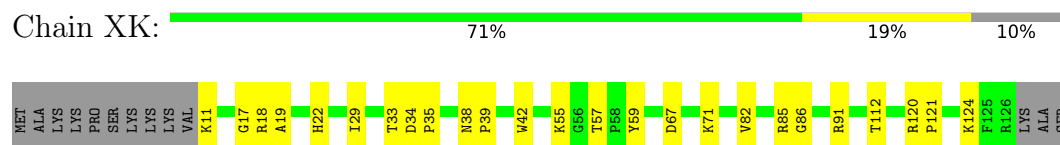
- Molecule 10: 30S ribosomal protein S10



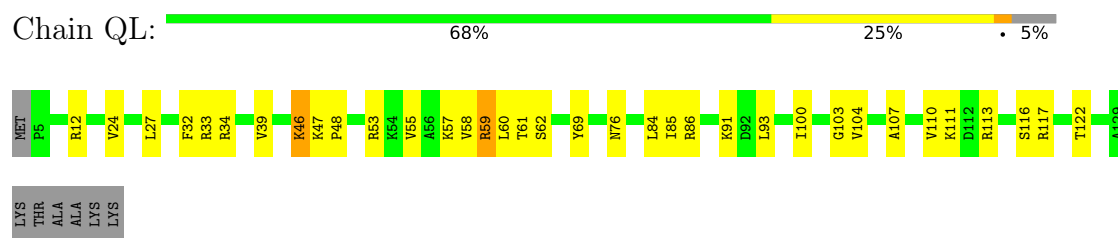
- Molecule 11: 30S ribosomal protein S11



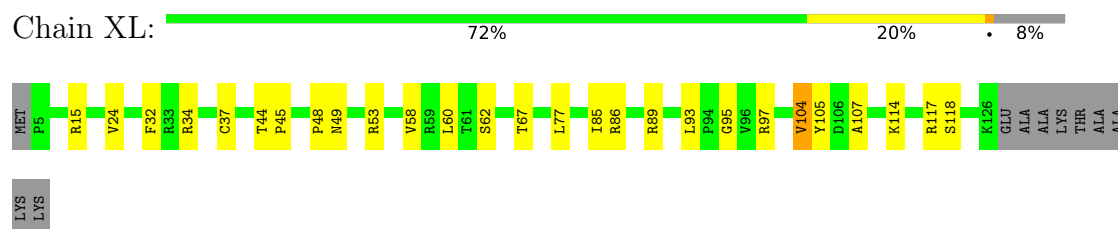
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

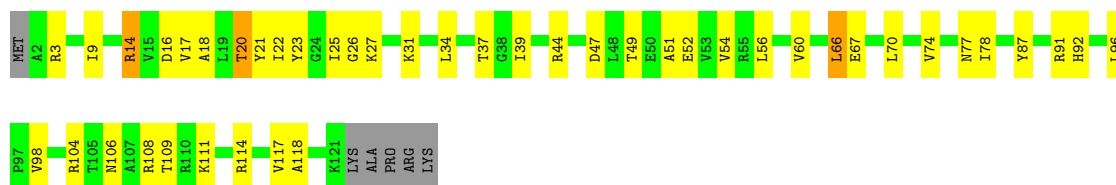


- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

Chain QM:  60% 33% • 5%



- Molecule 13: 30S ribosomal protein S13

Chain XM:  67% 25% • 6%



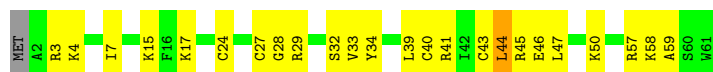
- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  70% 25% • •




- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  59% 38% • •




- Molecule 15: 30S ribosomal protein S15

Chain QO:  75% 24% •




- Molecule 15: 30S ribosomal protein S15

Chain XO:  80% 18% •




- Molecule 16: 30S ribosomal protein S16

Chain QP:  78% 17% 5%




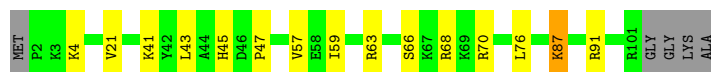
- Molecule 16: 30S ribosomal protein S16

Chain XP:  84% 11% 5%




- Molecule 17: 30S ribosomal protein S17

Chain QQ:  81% 13% 5%



- Molecule 17: 30S ribosomal protein S17

Chain XQ:  74% 20% 5%



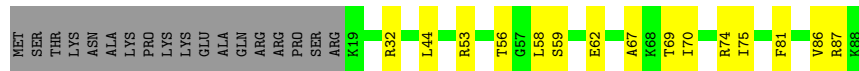
- Molecule 18: 30S ribosomal protein S18

Chain QR:  63% 17% 20%



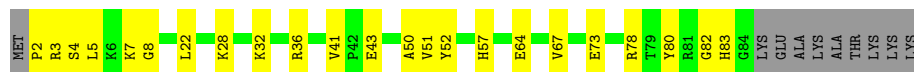
- Molecule 18: 30S ribosomal protein S18

Chain XR:  63% 17% 20%



- Molecule 19: 30S ribosomal protein S19

Chain QS:  65% 25% 11%




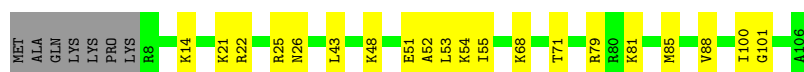
- Molecule 19: 30S ribosomal protein S19

Chain XS:  73% 17% 10%



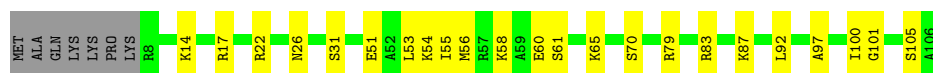
- Molecule 20: 30S ribosomal protein S20

Chain QT:  75% 19% 7%




- Molecule 20: 30S ribosomal protein S20

Chain XT:  72% 22% 7%



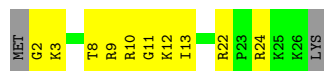
- Molecule 21: 30S ribosomal protein Thx

Chain QU:  74% 19% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain XU:  56% 37% 7%



- Molecule 22: P-site ASLPro

Chain QV:  52% 35% 13%



- Molecule 22: P-site ASLPro

Chain XV:  58% 26% 16%



- Molecule 23: mRNA

Chain QX:  32% 53% 11% 5%



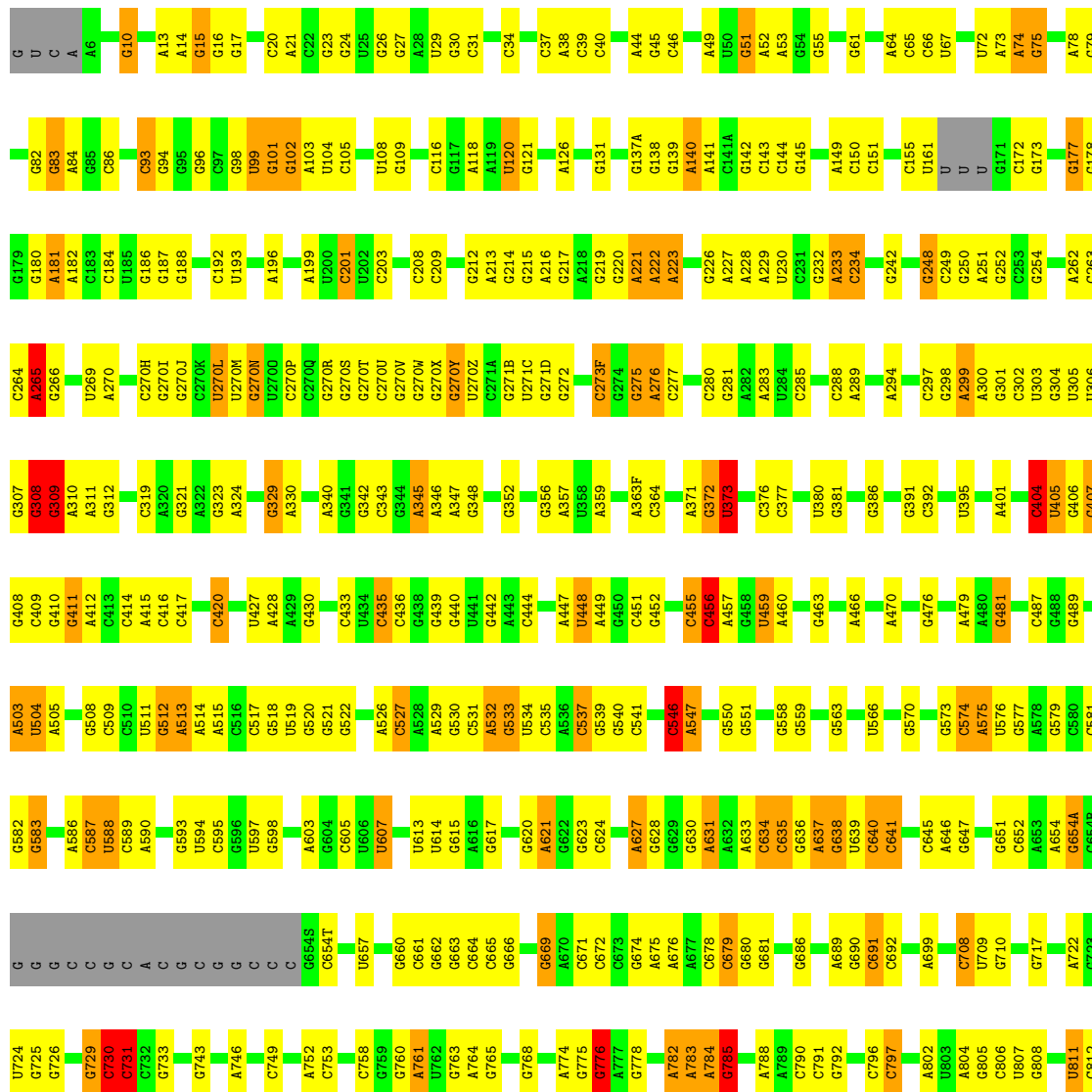
• Molecule 23: mRNA

Chain XX:  37% 58% 5%



• Molecule 24: 23S rRNA

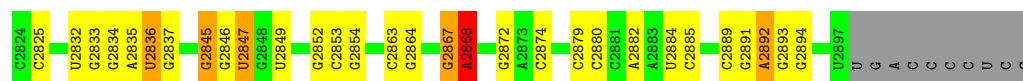
Chain RA:  49% 39% 10% ..



| | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|
| A2019 | A1923 | G1822 | A1732 | G1539 | C1467 | U1391 | C1297 | U1211 | A1054 | G975 | C976 | C977 | C815 |
| A2020 | C1924 | G1823 | G1733 | G1540 | C1468 | A1392 | C1298 | G1212 | A1055 | C976 | C976 | C976 | C816 |
| C2021 | A1927 | G1824 | C1742 | U1541 | A1469 | A1393 | G1299 | G1216 | G1056 | A980 | A980 | A980 | C817 |
| U2022 | A1928 | G1825 | G1743 | G1542 | G1470 | A1394 | U1300 | G1216 | A1057 | A980 | A980 | A980 | C818 |
| G2023 | G1929 | G1826 | G1743 | A1543 | A1471 | A1395 | A1301 | A1220 | G1058 | A980 | A980 | A980 | G819 |
| C2025 | G1930 | C1827 | G1750 | C1544 | A1472 | A1396 | A1302 | C1221 | G1059 | A980 | A980 | A980 | A819 |
| C2026 | U1931 | G1830 | G1751 | A1545 | G1473 | U1397 | A1309 | A1221 | U1060 | A980 | A980 | A980 | U822 |
| A2030 | A1938 | G1831 | C1752 | A1546 | C1474 | C1398 | G1310 | G1224 | U1061 | A980 | A980 | A980 | G823 |
| G2032 | G1939 | C1832 | G1753 | C1547 | G1475 | C1399 | G1311 | C1225 | G1062 | A980 | A980 | A980 | G824 |
| A2033 | U1940 | G1833 | C1754 | C1548 | G1476 | G1400 | G1312 | G1226 | G1063 | A980 | A980 | A980 | A824 |
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| G2035 | G1942 | G1835 | U1756 | C1550 | G1478 | C1402 | G1314 | A1227 | U1065 | A980 | A980 | A980 | U828 |
| G2036 | C1947 | C1836 | U1757 | C1551 | U1482 | C1403 | C1315 | A1227 | U1066 | A980 | A980 | A980 | A829 |
| G2037 | U1947 | G1837 | G1758 | G1552 | G1483 | C1404 | C1316 | A1227 | U1066 | A980 | A980 | A980 | G830 |
| G2038 | A1950 | U1841 | A1762 | C1557 | G1484 | U1405 | A1317 | G1232 | A1070 | A980 | A980 | A980 | G831 |
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| G2041 | U1953 | G1844 | G1765 | G1560 | G1487 | C1409 | A1321 | G1235 | A1073 | A980 | A980 | A980 | G834 |
| G2042 | C1954 | C1845 | G1766 | G1561 | G1488 | C1410 | U1326 | G1236 | G1074 | A980 | A980 | A980 | A835 |
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| G2048 | U1960 | G1852 | G1776 | A1567 | A1497 | A1420 | U1336 | A1246 | U1082 | A980 | A980 | A980 | G848 |
| A2051 | U1961 | G1853 | G1777 | A1568 | U1498 | G1421 | G1337 | A1246 | U1083 | A980 | A980 | A980 | A849 |
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| G2053 | U1963 | G1855 | A1780 | G1570 | G1500 | G1423 | G1339 | A1246 | A1085 | A980 | A980 | A980 | A851 |
| G2054 | U1964 | G1856 | C1781 | A1571 | G1501 | U1424 | U1340 | A1246 | A1086 | A980 | A980 | A980 | G852 |
| G2055 | U1965 | G1857 | G1782 | A1572 | C1502 | A1425 | U1341 | A1246 | G1087 | A980 | A980 | A980 | C853 |
| G2056 | U1966 | G1858 | A1783 | A1573 | U1503 | G1426 | U1342 | A1246 | A1088 | A980 | A980 | A980 | C854 |
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| G2058 | U1968 | G1860 | U1785 | A1575 | U1505 | G1428 | U1344 | A1246 | U1090 | A980 | A980 | A980 | U856 |
| G2059 | U1969 | G1861 | G1786 | A1576 | C1506 | A1429 | U1345 | A1246 | U1091 | A980 | A980 | A980 | U857 |
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| G2061 | U1971 | G1863 | G1788 | A1578 | C1508 | A1431 | U1347 | A1246 | U1093 | A980 | A980 | A980 | U859 |
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| G2070 | U1980 | G1872 | G1797 | A1587 | C1517 | U1440 | U1356 | A1246 | U1102 | A980 | A980 | A980 | U868 |
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| G2074 | U1984 | G1876 | U1801 | A1591 | C1521 | A1444 | U1360 | A1246 | U1106 | A980 | A980 | A980 | G874 |
| G2075 | U1985 | G1877 | G1802 | A1592 | C1522 | U1445 | U1361 | A1246 | U1107 | A980 | A980 | A980 | U875 |
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| G2078 | U1988 | G1880 | U1805 | A1595 | C1525 | G1448 | U1364 | A1246 | U1110 | A980 | A980 | A980 | G878 |
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| G2081 | U1991 | G1883 | G1808 | A1598 | C1528 | U1451 | U1367 | A1246 | U1113 | A980 | A980 | A980 | U881 |
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| G2091 | U2001 | G1893 | G1818 | A1608 | C1538 | A1461 | U1377 | A1246 | U1123 | A980 | A980 | A980 | C891 |
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| G2097 | U2007 | G1899 | G1824 | A1614 | C1544 | U1467 | U1383 | A1246 | U1129 | A980 | A980 | A980 | U897 |
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| G2102 | U2012 | G1904 | U1829 | A1619 | C1549 | U1472 | U1388 | A1246 | U1134 | A980 | A980 | A980 | G901 |
| G2103 | U2013 | G1905 | G1830 | A1620 | C1550 | U1473 | U1389 | A1246 | U1135 | A980 | A980 | A980 | C902 |
| G2104 | U2014 | G1906 | U1831 | A1621 | C1551 | U1474 | U1390 | A1246 | U1136 | A980 | A980 | A980 | G903 |
| G2105 | U2015 | G1907 | G1832 | A1622 | C1552 | U1475 | U1391 | A1246 | U1137 | A980 | A980 | A980 | C904 |
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| G2107 | U2017 | G1909 | G1834 | A1624 | C1554 | U1477 | U1393 | A1246 | U1139 | A980 | A980 | A980 | C906 |
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| G2111 | U2021 | G1913 | G1838 | A1628 | C1558 | U1481 | U1397 | A1246 | U1143 | A980 | A980 | A980 | C910 |
| G2112 | U2022 | G1914 | U1839 | A1629 | C1559 | U1482 | U1398 | A1246 | U1144 | A980 | A980 | A980 | G911 |
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| G2114 | U2024 | G1916 | U1841 | A1631 | C1561 | U1484 | U1400 | A1246 | U1146 | A980 | A980 | A980 | G913 |
| G2115 | U2025 | G1917 | G1842 | A1632 | C1562 | U1485 | U1401 | A1246 | U1147 | A980 | A980 | A980 | C914 |
| G2116 | U2026 | G1918 | U1843 | A1633 | C1563 | U1486 | U1402 | A1246 | U1148 | A980 | A980 | A980 | G915 |
| G2117 | U2027 | G1919 | G1844 | A1634 | C1564 | U1487 | U1403 | A1246 | U1149 | A980 | A980 | A980 | C916 |
| G2118 | U2028 | G1920 | U1845 | A1635 | C1565 | U1488 | U1404 | A1246 | U1150 | A980 | A980 | A980 | A917 |
| G2119 | U2 | | | | | | | | | | | | |

| | | | | | | | | | | | | | | |
|-------|-------|-------|-------|--------|-------|------|------|------|------|---|-------|------|-------|-------|
| U1454 | C1375 | U1292 | A1210 | U1130 | G1056 | U963 | C884 | C814 | C731 | G | G600 | G520 | U427 | G326 |
| U1455 | C1376 | C1293 | U1211 | G1131 | A1057 | C964 | C885 | C815 | C731 | G | G600 | G521 | A428 | G327 |
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| A1460 | A1378 | C1297 | C1221 | G1136 | G1059 | C970 | A887 | C817 | G741 | C | G604 | C523 | G430 | G329 |
| C1461 | A1379 | C1298 | C1222 | G1137 | U1060 | C971 | C888 | G818 | G742 | C | U607 | U524 | U431 | A330 |
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| C1463 | G1385 | U1300 | G1225 | G1139 | G1062 | A973 | C890 | A820 | A746 | C | A609 | A526 | C433 | A332 |
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| C1467 | A1393 | C1306 | C1230 | U1142 | U1066 | C975 | A896 | U822 | C749 | C | A610 | A529 | U435 | G338 |
| U1471 | U1394 | G1309 | G1231 | A1142A | G1067 | C976 | A900 | U823 | A746 | C | G611 | G530 | U436 | U339 |
| C1474 | A1395 | G1310 | G1232 | A1143 | G1068 | A900 | U907 | U824 | A746 | C | U614 | G531 | A340 | A340 |
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| G1482 | C1397 | U1314 | U1234 | C1150 | A1070 | A900 | U907 | U826 | A746 | C | U614 | A533 | U359 | U359 |
| G1483 | C1398 | C1313 | G1235 | G1151 | G1071 | A900 | U907 | U827 | A746 | C | U614 | A534 | A359 | A359 |
| G1487 | C1399 | C1314 | U1236 | G1152 | G1072 | A900 | U907 | U828 | A746 | C | U614 | A535 | G363 | G363 |
| U1490 | G1400 | C1315 | A1237 | A1155 | A1073 | A900 | U907 | U829 | A746 | C | U614 | A536 | A363A | A363A |
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| U1496 | C1402 | A1317 | A1242 | A1157 | C1075 | A900 | U907 | U831 | A746 | C | U614 | A538 | A363C | A363C |
| U1497 | C1403 | G1324 | G1243 | C1158 | A1076 | A900 | U907 | U832 | A746 | C | U614 | A539 | A363D | A363D |
| C1498 | C1404 | G1325 | G1244 | C1159 | A1077 | A900 | U907 | U833 | A746 | C | U614 | A540 | A363E | A363E |
| G1500 | U1405 | U1325 | G1245 | U1159 | A1078 | A900 | U907 | U834 | A746 | C | U614 | A541 | A363F | A363F |
| C1504 | U1406 | U1326 | G1246 | G1160 | C1079 | A900 | U907 | U835 | A746 | C | U614 | A542 | A364 | A364 |
| C1505 | A1407 | U1327 | A1247 | A1161 | C1080 | A900 | U907 | U836 | A746 | C | U614 | A543 | A365 | A365 |
| C1506 | C1408 | G1332 | G1248 | A1162 | U1081 | A900 | U907 | U837 | A746 | C | U614 | A544 | A366 | A366 |
| C1507 | G1409 | C1333 | U1249 | G1163 | U1082 | A900 | U907 | U838 | A746 | C | U614 | A545 | A367 | A367 |
| C1508 | C1410 | G1334 | G1250 | C1164 | U1083 | A900 | U907 | U839 | A746 | C | U614 | A546 | A368 | A368 |
| C1509 | A1411 | U1335 | G1251 | U1165 | A1084 | A900 | U907 | U840 | A746 | C | U614 | A547 | A369 | A369 |
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| C1511 | U1416 | A1336 | G1253 | U1167 | A1086 | A900 | U907 | U842 | A746 | C | U614 | A549 | A371 | A371 |
| C1512 | C1417 | G1337 | A1254 | G1168 | C1087 | A900 | U907 | U843 | A746 | C | U614 | A550 | A372 | A372 |
| C1513 | G1418 | U1338 | U1255 | G1169 | A1088 | A900 | U907 | U844 | A746 | C | U614 | A551 | A373 | A373 |
| C1514 | A1419 | U1339 | G1256 | G1170 | U1089 | A900 | U907 | U845 | A746 | C | U614 | A552 | A374 | A374 |
| C1515 | U1420 | U1340 | C1257 | C1171 | G1090 | A900 | U907 | U846 | A746 | C | U614 | A553 | A375 | A375 |
| C1516 | G1421 | A1341 | U1258 | U1172 | U1091 | A900 | U907 | U847 | A746 | C | U614 | A554 | A376 | A376 |
| C1517 | C1422 | G1342 | G1259 | C1173 | U1092 | A900 | U907 | U848 | A746 | C | U614 | A555 | A377 | A377 |
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| C1520 | U1425 | C1345 | A1262 | C1176 | A1095 | A900 | U907 | U851 | A746 | C | U614 | A558 | A380 | A380 |
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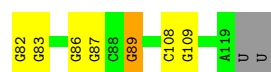
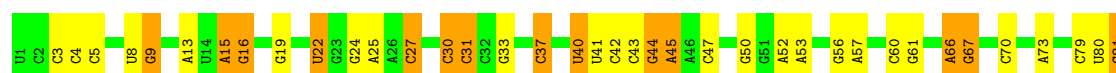
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| | | C2694 | C2415 | C2415 | C2415 | G2417 | G2256 | C2171 | C2098 | | U1913 | | | |
| | | C2695 | C2416 | C2416 | C2416 | G2418 | G2257 | C2172 | C2099 | | U1914 | | | |
| | | C2696 | C2417 | C2417 | C2417 | G2419 | G2258 | C2173 | C2100 | | U1915 | | | |
| | | C2697 | C2418 | C2418 | C2418 | G2420 | G2259 | C2174 | C2101 | | U1916 | | | |
| | | C2698 | C2419 | C2419 | C2419 | G2421 | G2260 | C2175 | C2102 | | U1917 | | | |
| | | C2699 | C2420 | C2420 | C2420 | G2422 | G2261 | C2176 | C2103 | | U1918 | | | |
| | | C2700 | C2421 | C2421 | C2421 | G2423 | G2262 | C2177 | C2104 | | U1919 | | | |



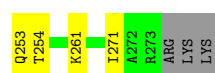
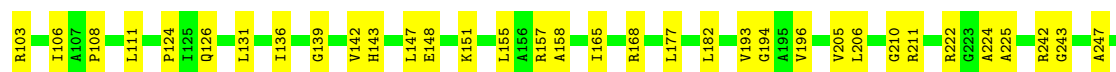
• Molecule 25: 5S rRNA



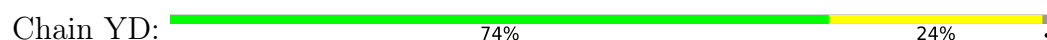
• Molecule 25: 5S rRNA



• Molecule 26: 50S ribosomal protein L2

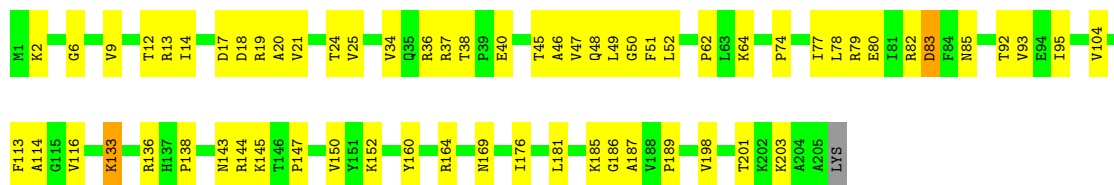


• Molecule 26: 50S ribosomal protein L2



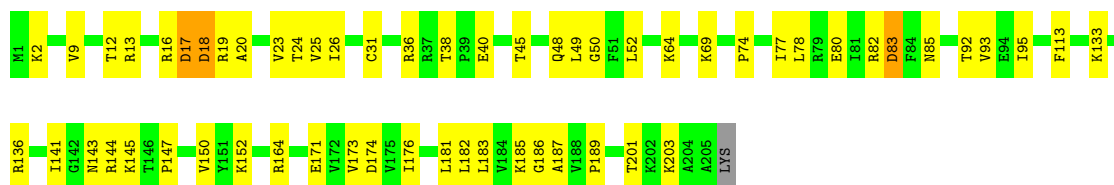
• Molecule 27: 50S ribosomal protein L3

Chain RE:  68% 30% .




- Molecule 27: 50S ribosomal protein L3

Chain YE:  71% 27% .




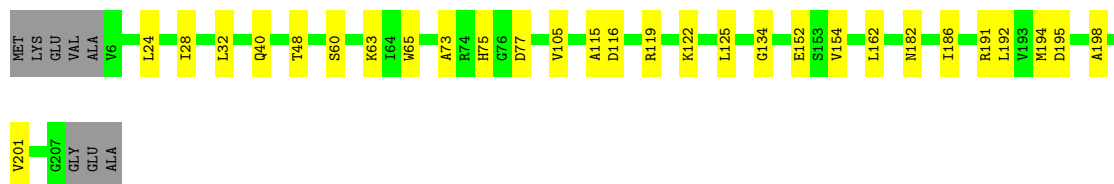
- Molecule 28: 50S ribosomal protein L4

Chain RF:  81% 15% .




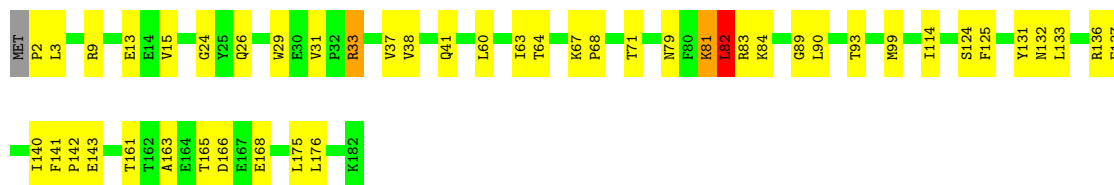
- Molecule 28: 50S ribosomal protein L4

Chain YF:  82% 14% .



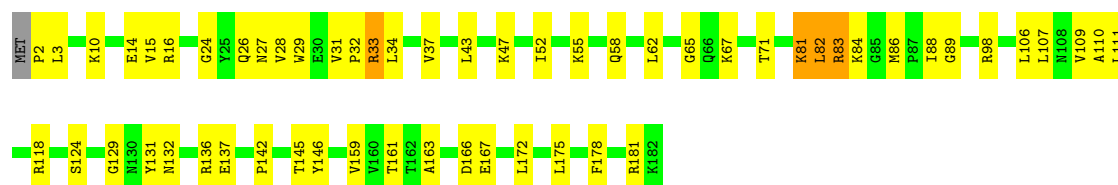
- Molecule 29: 50S ribosomal protein L5

Chain RG:  74% 24% ...



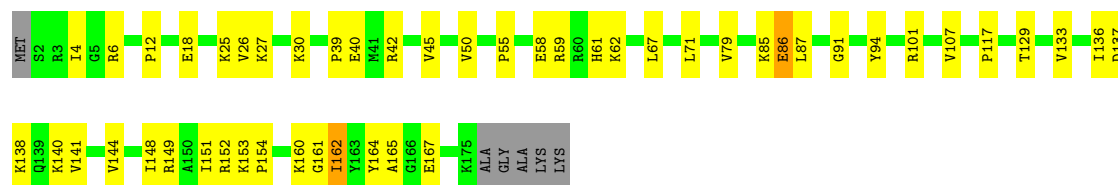
- Molecule 29: 50S ribosomal protein L5

Chain YG:  68% 29% ..




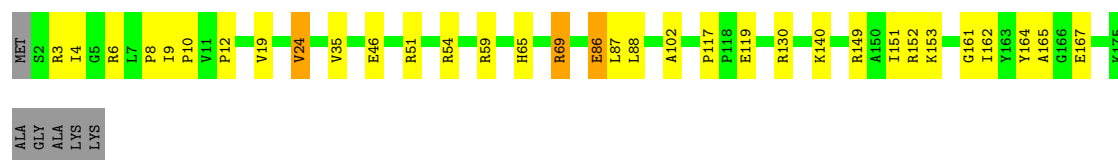
- Molecule 30: 50S ribosomal protein L6

Chain RH:  69% 26% ..




- Molecule 30: 50S ribosomal protein L6


Chain YH:  78% 17% ..



- Molecule 31: 50S ribosomal protein L9


Chain RI:  82% 16% ..



Chain YN:  80% 18% ..




- Molecule 33: 50S ribosomal protein L14

Chain RO:  74% 26%



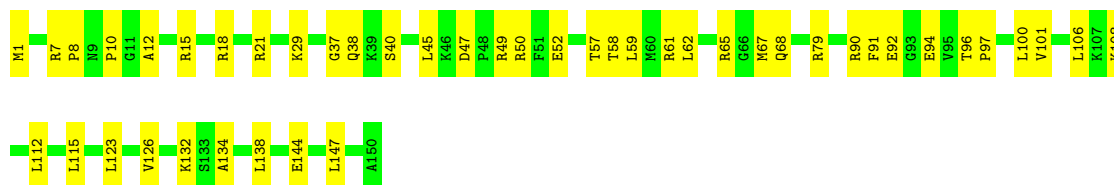
- Molecule 33: 50S ribosomal protein L14

Chain YO:  80% 20%




- Molecule 34: 50S ribosomal protein L15

Chain RP:  70% 30%




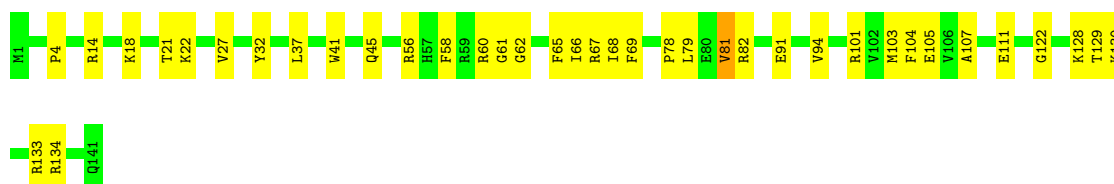
- Molecule 34: 50S ribosomal protein L15

Chain YP:  75% 23% .

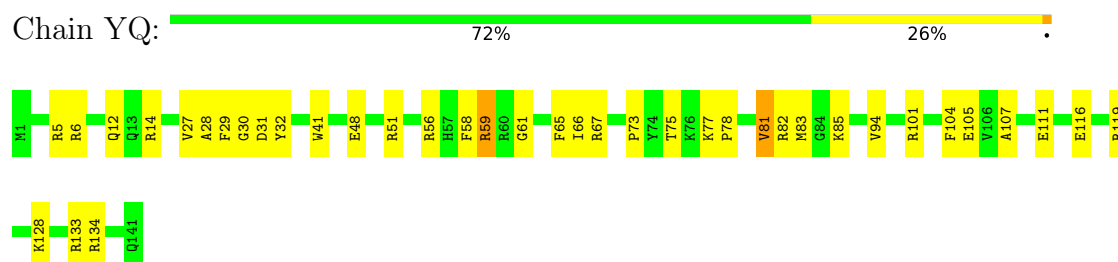


- Molecule 35: 50S ribosomal protein L16

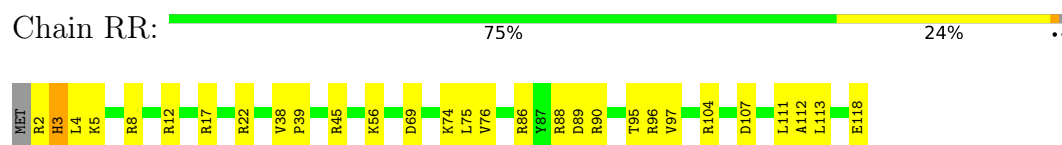
Chain RQ:  73% 26% .



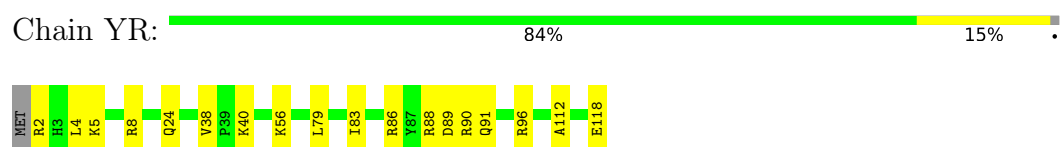
• Molecule 35: 50S ribosomal protein L16



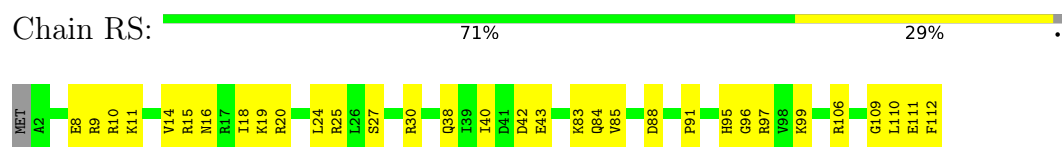
• Molecule 36: 50S ribosomal protein L17



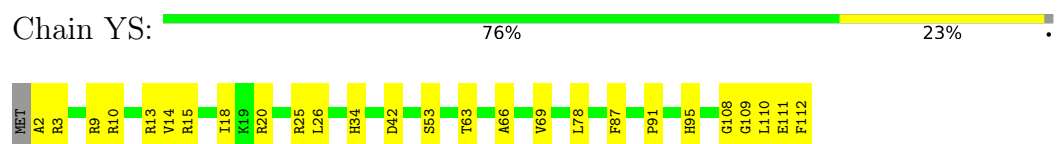
• Molecule 36: 50S ribosomal protein L17



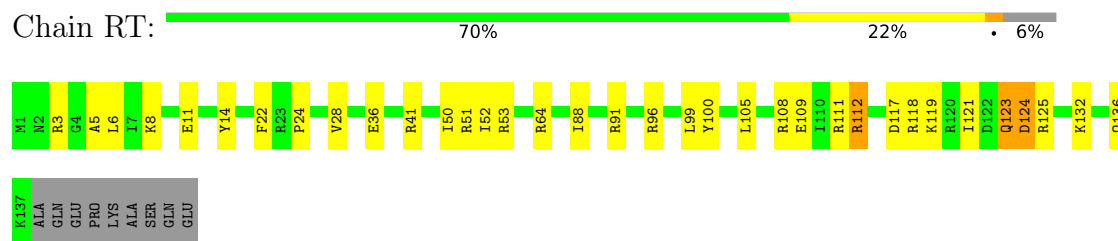
• Molecule 37: 50S ribosomal protein L18



• Molecule 37: 50S ribosomal protein L18

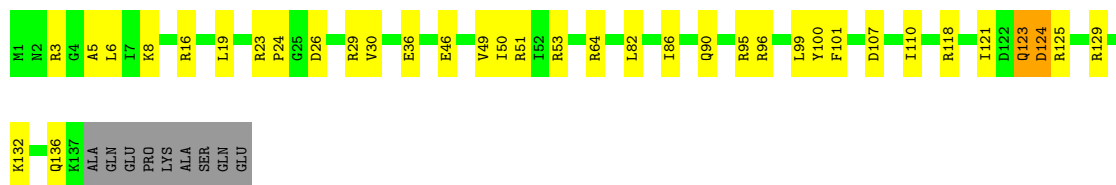


• Molecule 38: 50S ribosomal protein L19




• Molecule 38: 50S ribosomal protein L19

Chain YT:  69% 23% 6%




- Molecule 39: 50S ribosomal protein L20

Chain RU:  85% 13% ..




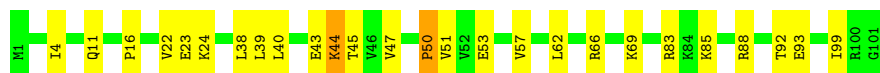
- Molecule 39: 50S ribosomal protein L20

Chain YU:  81% 17% ..




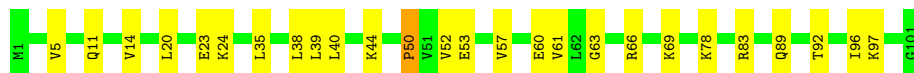
- Molecule 40: 50S ribosomal protein L21

Chain RV:  74% 24% .




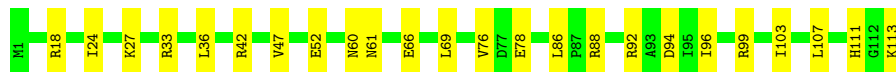
- Molecule 40: 50S ribosomal protein L21

Chain YV:  74% 25% .



- Molecule 41: 50S ribosomal protein L22

Chain RW:  79% 21%




- Molecule 41: 50S ribosomal protein L22

Chain YW:  85% 14% .




- Molecule 42: 50S ribosomal protein L23

Chain RX:  82% 14% .




- Molecule 42: 50S ribosomal protein L23

Chain YX:  81% 15% .



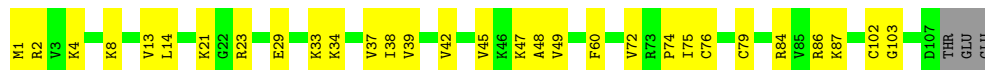
- Molecule 43: 50S ribosomal protein L24

Chain RY:  75% 22% .



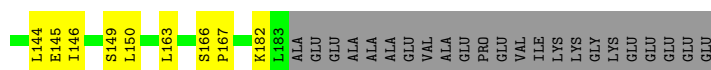
- Molecule 43: 50S ribosomal protein L24

Chain YY:  70% 27% .



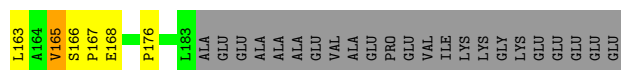
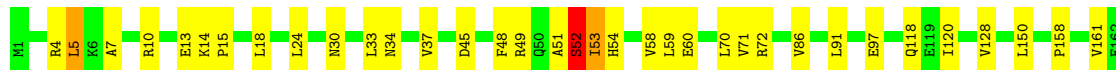
- Molecule 44: 50S ribosomal protein L25

Chain RZ:  67% 21% 11%




- Molecule 44: 50S ribosomal protein L25

Chain YZ:  69% 18% 11%



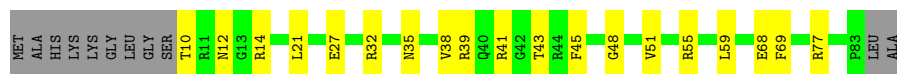
- Molecule 45: 50S ribosomal protein L27

Chain R0:  75% 20% 5%




- Molecule 45: 50S ribosomal protein L27

Chain Y0:  65% 22% 13%




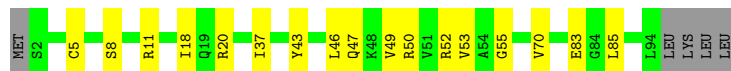
- Molecule 46: 50S ribosomal protein L28

Chain R1:  81% 18% .



- Molecule 46: 50S ribosomal protein L28

Chain Y1:  78% 17% 5%




- Molecule 47: 50S ribosomal protein L29

Chain R2:  72% 24% .




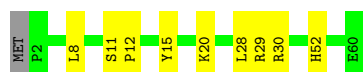
- Molecule 47: 50S ribosomal protein L29

Chain Y2:  74% 22% .




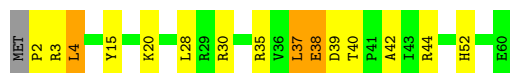
- Molecule 48: 50S ribosomal protein L30

Chain R3:  83% 15% .



- Molecule 48: 50S ribosomal protein L30

Chain Y3:  73% 20% 5% .



- Molecule 49: 50S ribosomal protein L31

Chain R4:  72% 25% .



- Molecule 49: 50S ribosomal protein L31

Chain Y4:  58% 37% . .




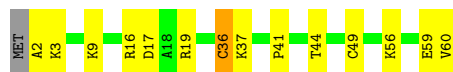
- Molecule 50: 50S ribosomal protein L32

Chain R5:  72% 27% .




- Molecule 50: 50S ribosomal protein L32

Chain Y5:  75% 22% . .



- Molecule 51: 50S ribosomal protein L33

Chain R6:  80% 19% .




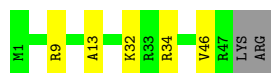
- Molecule 51: 50S ribosomal protein L33

Chain Y6:  67% 31% .




- Molecule 52: 50S ribosomal protein L34

Chain R7:  86% 10% .



- Molecule 52: 50S ribosomal protein L34

Chain Y7:  82% 16% .



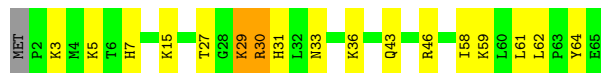
- Molecule 53: 50S ribosomal protein L35

Chain R8:  68% 28% . .



- Molecule 53: 50S ribosomal protein L35

Chain Y8:  72% 23% . .




- Molecule 54: 50S ribosomal protein L36

Chain R9:  70% 30%



- Molecule 54: 50S ribosomal protein L36

Chain Y9:  84% 16%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 209.97Å 450.71Å 619.40Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.82 – 3.97 | Depositor |
| % Data completeness (in resolution range) | 98.7 (49.82-3.97) | Depositor |
| R_{merge} | 0.33 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.36 (at 4.00Å) | Xtriage |
| Refinement program | PHENIX 1.14_3260 | Depositor |
| R, R_{free} | 0.228 , 0.255 | Depositor |
| Wilson B-factor (Å ²) | 146.0 | Xtriage |
| Anisotropy | 0.246 | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 291782 | wwPDB-VP |
| Average B, all atoms (Å ²) | 177.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | QA | 0.59 | 0/36098 | 1.09 | 116/56341 (0.2%) |
| 1 | XA | 0.59 | 0/36101 | 1.09 | 126/56346 (0.2%) |
| 2 | QB | 0.44 | 0/1942 | 0.69 | 1/2619 (0.0%) |
| 2 | XB | 0.46 | 0/1950 | 0.68 | 0/2630 |
| 3 | QC | 0.46 | 0/1629 | 0.72 | 0/2195 |
| 3 | XC | 0.44 | 0/1629 | 0.72 | 0/2195 |
| 4 | QD | 0.47 | 1/1733 (0.1%) | 0.67 | 0/2318 |
| 4 | XD | 0.53 | 1/1733 (0.1%) | 0.65 | 0/2318 |
| 5 | QE | 0.46 | 1/1171 (0.1%) | 0.68 | 1/1576 (0.1%) |
| 5 | XE | 0.45 | 0/1171 | 0.69 | 0/1576 |
| 6 | QF | 0.46 | 0/856 | 0.69 | 0/1154 |
| 6 | XF | 0.41 | 0/856 | 0.66 | 0/1154 |
| 7 | QG | 0.46 | 0/1276 | 0.67 | 0/1709 |
| 7 | XG | 0.45 | 0/1276 | 0.70 | 0/1709 |
| 8 | QH | 0.45 | 0/1128 | 0.64 | 1/1517 (0.1%) |
| 8 | XH | 0.41 | 0/1128 | 0.63 | 0/1517 |
| 9 | QI | 0.46 | 0/1008 | 0.77 | 3/1354 (0.2%) |
| 9 | XI | 0.45 | 0/1017 | 0.79 | 2/1365 (0.1%) |
| 10 | QJ | 0.45 | 0/814 | 0.69 | 1/1095 (0.1%) |
| 10 | XJ | 0.46 | 0/790 | 0.71 | 0/1063 |
| 11 | QK | 0.42 | 0/900 | 0.59 | 0/1213 |
| 11 | XK | 0.42 | 0/879 | 0.66 | 0/1187 |
| 12 | QL | 0.44 | 0/991 | 0.69 | 0/1327 |
| 12 | XL | 0.43 | 0/972 | 0.70 | 0/1301 |
| 13 | QM | 0.46 | 0/965 | 0.74 | 0/1292 |
| 13 | XM | 0.49 | 0/956 | 0.83 | 1/1281 (0.1%) |
| 14 | QN | 0.42 | 0/501 | 0.70 | 1/664 (0.2%) |
| 14 | XN | 0.51 | 0/501 | 0.76 | 1/664 (0.2%) |
| 15 | QO | 0.40 | 0/745 | 0.56 | 0/992 |
| 15 | XO | 0.41 | 0/740 | 0.62 | 0/987 |
| 16 | QP | 0.46 | 0/721 | 0.63 | 0/970 |
| 16 | XP | 0.43 | 0/721 | 0.70 | 0/970 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | QQ | 0.38 | 0/847 | 0.61 | 0/1131 |
| 17 | XQ | 0.39 | 0/847 | 0.63 | 0/1131 |
| 18 | QR | 0.40 | 0/579 | 0.61 | 0/768 |
| 18 | XR | 0.44 | 0/579 | 0.65 | 0/768 |
| 19 | QS | 0.39 | 0/680 | 0.74 | 1/915 (0.1%) |
| 19 | XS | 0.46 | 0/689 | 0.75 | 0/926 |
| 20 | QT | 0.37 | 0/765 | 0.61 | 0/1007 |
| 20 | XT | 0.49 | 0/765 | 0.75 | 0/1007 |
| 21 | QU | 0.41 | 0/221 | 0.68 | 0/288 |
| 21 | XU | 0.40 | 0/221 | 0.71 | 0/288 |
| 22 | QV | 0.47 | 1/1840 (0.1%) | 1.02 | 6/2866 (0.2%) |
| 22 | XV | 0.42 | 1/1840 (0.1%) | 1.02 | 9/2866 (0.3%) |
| 23 | QX | 0.28 | 0/470 | 0.86 | 1/733 (0.1%) |
| 23 | XX | 0.33 | 0/470 | 0.90 | 0/733 |
| 24 | RA | 0.76 | 1/69521 (0.0%) | 1.14 | 353/108529 (0.3%) |
| 24 | YA | 0.89 | 3/69543 (0.0%) | 1.17 | 381/108563 (0.4%) |
| 25 | RB | 0.56 | 0/2878 | 1.14 | 22/4490 (0.5%) |
| 25 | YB | 0.78 | 0/2878 | 1.19 | 15/4490 (0.3%) |
| 26 | RD | 0.51 | 0/2165 | 0.71 | 2/2919 (0.1%) |
| 26 | YD | 0.53 | 0/2165 | 0.68 | 2/2919 (0.1%) |
| 27 | RE | 0.45 | 0/1601 | 0.72 | 0/2160 |
| 27 | YE | 0.47 | 0/1601 | 0.68 | 0/2160 |
| 28 | RF | 0.49 | 0/1620 | 0.64 | 0/2194 |
| 28 | YF | 0.55 | 0/1620 | 0.66 | 0/2194 |
| 29 | RG | 0.44 | 0/1499 | 0.73 | 0/2016 |
| 29 | YG | 0.46 | 0/1499 | 0.73 | 0/2016 |
| 30 | RH | 0.48 | 0/1362 | 0.75 | 0/1841 |
| 30 | YH | 0.49 | 0/1362 | 0.74 | 0/1841 |
| 31 | RI | 0.43 | 0/1151 | 0.76 | 0/1558 |
| 31 | YI | 0.46 | 0/1151 | 0.76 | 1/1558 (0.1%) |
| 32 | RN | 0.42 | 0/1131 | 0.67 | 0/1525 |
| 32 | YN | 0.50 | 0/1131 | 0.69 | 0/1525 |
| 33 | RO | 0.52 | 0/943 | 0.67 | 0/1269 |
| 33 | YO | 0.51 | 0/943 | 0.67 | 0/1269 |
| 34 | RP | 0.47 | 0/1162 | 0.78 | 0/1544 |
| 34 | YP | 0.47 | 0/1139 | 0.73 | 0/1514 |
| 35 | RQ | 0.45 | 0/1143 | 0.70 | 0/1527 |
| 35 | YQ | 0.51 | 0/1143 | 0.71 | 0/1527 |
| 36 | RR | 0.45 | 0/974 | 0.67 | 0/1302 |
| 36 | YR | 0.46 | 0/974 | 0.67 | 0/1302 |
| 37 | RS | 0.43 | 0/892 | 0.76 | 0/1187 |
| 37 | YS | 0.44 | 0/892 | 0.72 | 0/1187 |
| 38 | RT | 0.46 | 0/1155 | 0.75 | 2/1542 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | YT | 0.48 | 0/1155 | 0.74 | 2/1542 (0.1%) |
| 39 | RU | 0.46 | 0/982 | 0.65 | 0/1306 |
| 39 | YU | 0.55 | 0/982 | 0.64 | 0/1306 |
| 40 | RV | 0.48 | 0/790 | 0.72 | 0/1057 |
| 40 | YV | 0.49 | 0/790 | 0.70 | 0/1057 |
| 41 | RW | 0.50 | 0/911 | 0.67 | 0/1220 |
| 41 | YW | 0.50 | 0/911 | 0.64 | 0/1220 |
| 42 | RX | 0.43 | 0/739 | 0.64 | 1/993 (0.1%) |
| 42 | YX | 0.50 | 0/739 | 0.67 | 1/993 (0.1%) |
| 43 | RY | 0.44 | 0/831 | 0.60 | 0/1108 |
| 43 | YY | 0.46 | 0/831 | 0.58 | 0/1108 |
| 44 | RZ | 0.49 | 0/1493 | 0.79 | 0/2026 |
| 44 | YZ | 0.44 | 0/1493 | 0.74 | 2/2026 (0.1%) |
| 45 | R0 | 0.41 | 0/652 | 0.61 | 0/867 |
| 45 | Y0 | 0.44 | 0/601 | 0.60 | 0/801 |
| 46 | R1 | 0.46 | 0/770 | 0.66 | 0/1022 |
| 46 | Y1 | 0.50 | 0/736 | 0.69 | 0/978 |
| 47 | R2 | 0.49 | 0/583 | 0.68 | 0/771 |
| 47 | Y2 | 0.46 | 0/583 | 0.68 | 0/771 |
| 48 | R3 | 0.43 | 0/474 | 0.65 | 0/635 |
| 48 | Y3 | 0.49 | 0/474 | 0.66 | 0/635 |
| 49 | R4 | 0.44 | 0/578 | 0.73 | 0/776 |
| 49 | Y4 | 0.48 | 0/578 | 0.76 | 0/776 |
| 50 | R5 | 0.46 | 0/473 | 0.62 | 0/639 |
| 50 | Y5 | 0.50 | 0/473 | 0.78 | 1/639 (0.2%) |
| 51 | R6 | 0.40 | 0/460 | 0.60 | 0/613 |
| 51 | Y6 | 0.45 | 0/460 | 0.62 | 0/613 |
| 52 | R7 | 0.44 | 0/417 | 0.65 | 0/550 |
| 52 | Y7 | 0.49 | 0/426 | 0.64 | 0/561 |
| 53 | R8 | 0.52 | 0/525 | 0.75 | 0/691 |
| 53 | Y8 | 0.59 | 0/525 | 0.76 | 0/691 |
| 54 | R9 | 0.37 | 0/310 | 0.62 | 0/407 |
| 54 | Y9 | 0.42 | 0/310 | 0.59 | 0/407 |
| All | All | 0.68 | 9/316004 (0.0%) | 1.03 | 1056/472499 (0.2%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 4 | QD | 0 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 12 | XL | 0 | 1 |
| 27 | YE | 0 | 1 |
| 29 | RG | 0 | 1 |
| 29 | YG | 0 | 1 |
| 44 | RZ | 0 | 1 |
| 44 | YZ | 0 | 1 |
| All | All | 0 | 7 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|--------|--------|-------------|----------|
| 4 | XD | 61 | LYS | CE-NZ | 11.17 | 1.76 | 1.49 |
| 22 | QV | 1 | C | OP3-P | -10.43 | 1.48 | 1.61 |
| 22 | XV | 1 | C | OP3-P | -10.41 | 1.48 | 1.61 |
| 4 | QD | 13 | ARG | CZ-NH1 | 7.36 | 1.42 | 1.33 |
| 5 | QE | 57 | LYS | CD-CE | 5.31 | 1.64 | 1.51 |
| 24 | RA | 248 | G | N7-C5 | -5.28 | 1.36 | 1.39 |
| 24 | YA | 2712(A) | A | N9-C8 | -5.24 | 1.33 | 1.37 |
| 24 | YA | 2712(A) | A | N7-C5 | -5.14 | 1.36 | 1.39 |
| 24 | YA | 2868 | A | N7-C5 | -5.10 | 1.36 | 1.39 |

All (1056) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 24 | RA | 1774 | C | C2-N1-C1' | 19.55 | 140.31 | 118.80 |
| 24 | RA | 1774 | C | C6-N1-C1' | -15.44 | 102.27 | 120.80 |
| 1 | XA | 359 | U | C2-N1-C1' | 13.62 | 134.05 | 117.70 |
| 24 | YA | 1158 | C | C2-N1-C1' | 13.17 | 133.29 | 118.80 |
| 1 | QA | 1301 | U | N1-C2-O2 | 12.01 | 131.21 | 122.80 |
| 24 | YA | 1313 | U | N3-C2-O2 | -11.93 | 113.85 | 122.20 |
| 24 | YA | 511 | U | C2-N1-C1' | 11.92 | 132.01 | 117.70 |
| 24 | YA | 856 | C | C6-N1-C2 | -11.75 | 115.60 | 120.30 |
| 50 | Y5 | 60 | VAL | CA-C-O | -11.67 | 95.59 | 120.10 |
| 25 | RB | 31 | C | N1-C2-O2 | 11.35 | 125.71 | 118.90 |
| 24 | RA | 1774 | C | N3-C2-O2 | -11.34 | 113.96 | 121.90 |
| 24 | YA | 1158 | C | C6-N1-C1' | -10.95 | 107.66 | 120.80 |
| 24 | RA | 856 | C | C6-N1-C2 | -10.93 | 115.93 | 120.30 |
| 24 | YA | 1535 | U | N1-C2-O2 | 10.68 | 130.27 | 122.80 |
| 1 | XA | 359 | U | C6-N1-C1' | -10.61 | 106.35 | 121.20 |
| 1 | QA | 1301 | U | N3-C2-O2 | -10.60 | 114.78 | 122.20 |
| 1 | QA | 328 | C | N1-C2-O2 | 10.52 | 125.21 | 118.90 |
| 1 | QA | 1158 | C | N1-C2-O2 | 10.47 | 125.18 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|--------|-------------|----------|
| 24 | YA | 2712(A) | A | N7-C8-N9 | 10.45 | 119.03 | 113.80 |
| 24 | RA | 546 | C | N1-C2-O2 | 10.38 | 125.13 | 118.90 |
| 1 | XA | 1158 | C | N1-C2-O2 | 10.35 | 125.11 | 118.90 |
| 24 | YA | 2868 | A | N7-C8-N9 | 10.35 | 118.97 | 113.80 |
| 1 | XA | 328 | C | N1-C2-O2 | 10.32 | 125.09 | 118.90 |
| 24 | RA | 1774 | C | N1-C2-O2 | 10.29 | 125.07 | 118.90 |
| 24 | YA | 2868 | A | C8-N9-C4 | -10.17 | 101.73 | 105.80 |
| 24 | YA | 1313 | U | N1-C2-O2 | 10.11 | 129.88 | 122.80 |
| 25 | YB | 31 | C | N1-C2-O2 | 9.96 | 124.88 | 118.90 |
| 24 | RA | 1968 | G | C4-N9-C1' | 9.87 | 139.33 | 126.50 |
| 24 | YA | 1407 | C | C6-N1-C2 | -9.80 | 116.38 | 120.30 |
| 1 | QA | 1158 | C | N3-C2-O2 | -9.67 | 115.13 | 121.90 |
| 24 | RA | 308 | G | C8-N9-C1' | 9.65 | 139.55 | 127.00 |
| 24 | YA | 1535 | U | N3-C2-O2 | -9.65 | 115.44 | 122.20 |
| 24 | YA | 1313 | U | C2-N1-C1' | 9.65 | 129.28 | 117.70 |
| 24 | RA | 1968 | G | C8-N9-C1' | -9.57 | 114.56 | 127.00 |
| 24 | YA | 120 | U | N3-C2-O2 | -9.53 | 115.53 | 122.20 |
| 24 | RA | 308 | G | C4-N9-C1' | -9.50 | 114.14 | 126.50 |
| 24 | YA | 511 | U | C6-N1-C1' | -9.48 | 107.93 | 121.20 |
| 24 | YA | 1956 | U | N3-C2-O2 | -9.46 | 115.58 | 122.20 |
| 24 | YA | 1774 | C | N3-C2-O2 | -9.34 | 115.36 | 121.90 |
| 24 | YA | 860 | U | N3-C2-O2 | -9.29 | 115.70 | 122.20 |
| 24 | YA | 1670 | C | C2-N1-C1' | 9.20 | 128.92 | 118.80 |
| 24 | RA | 1313 | U | N3-C2-O2 | -9.18 | 115.78 | 122.20 |
| 1 | QA | 1158 | C | C6-N1-C2 | -9.17 | 116.63 | 120.30 |
| 24 | RA | 2666 | C | N1-C2-O2 | 9.15 | 124.39 | 118.90 |
| 24 | RA | 1640 | C | N1-C2-O2 | 9.08 | 124.35 | 118.90 |
| 24 | RA | 120 | U | N3-C2-O2 | -9.07 | 115.85 | 122.20 |
| 24 | RA | 373 | U | N3-C2-O2 | -8.97 | 115.92 | 122.20 |
| 24 | YA | 828 | U | C2-N1-C1' | 8.93 | 128.41 | 117.70 |
| 24 | YA | 1914 | C | N1-C2-O2 | 8.84 | 124.20 | 118.90 |
| 1 | XA | 330 | C | N1-C2-O2 | 8.76 | 124.16 | 118.90 |
| 24 | YA | 856 | C | C5-C6-N1 | 8.75 | 125.37 | 121.00 |
| 24 | YA | 1774 | C | N1-C2-O2 | 8.70 | 124.12 | 118.90 |
| 24 | YA | 1968 | G | O4'-C1'-N9 | 8.66 | 115.12 | 108.20 |
| 24 | YA | 1968 | G | C4-N9-C1' | 8.64 | 137.74 | 126.50 |
| 24 | RA | 373 | U | N1-C2-O2 | 8.64 | 128.85 | 122.80 |
| 24 | RA | 1956 | U | N3-C2-O2 | -8.57 | 116.20 | 122.20 |
| 1 | XA | 979 | C | N1-C2-O2 | 8.51 | 124.01 | 118.90 |
| 25 | YB | 31 | C | C2-N1-C1' | 8.51 | 128.16 | 118.80 |
| 24 | RA | 120 | U | N1-C2-O2 | 8.49 | 128.74 | 122.80 |
| 1 | QA | 328 | C | N3-C2-O2 | -8.48 | 115.96 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24 | RA | 1914 | C | N1-C2-O2 | 8.47 | 123.98 | 118.90 |
| 1 | XA | 1158 | C | N3-C2-O2 | -8.44 | 115.99 | 121.90 |
| 24 | RA | 828 | U | N1-C2-O2 | 8.44 | 128.71 | 122.80 |
| 24 | RA | 546 | C | N3-C2-O2 | -8.43 | 116.00 | 121.90 |
| 25 | YB | 37 | C | N1-C2-O2 | 8.41 | 123.95 | 118.90 |
| 1 | XA | 358 | U | N1-C1'-C2' | -8.38 | 102.79 | 112.00 |
| 24 | RA | 1931 | U | N1-C2-O2 | 8.36 | 128.65 | 122.80 |
| 24 | RA | 828 | U | N3-C2-O2 | -8.35 | 116.35 | 122.20 |
| 1 | XA | 328 | C | N3-C2-O2 | -8.35 | 116.06 | 121.90 |
| 24 | YA | 2814 | C | N3-C2-O2 | -8.35 | 116.06 | 121.90 |
| 24 | YA | 1159 | U | C2-N1-C1' | 8.34 | 127.71 | 117.70 |
| 1 | QA | 1322 | C | N1-C2-O2 | 8.33 | 123.90 | 118.90 |
| 24 | YA | 1407 | C | C5-C6-N1 | 8.32 | 125.16 | 121.00 |
| 24 | YA | 120 | U | N1-C2-O2 | 8.31 | 128.61 | 122.80 |
| 24 | YA | 1968 | G | C8-N9-C1' | -8.26 | 116.26 | 127.00 |
| 25 | RB | 31 | C | N3-C2-O2 | -8.26 | 116.12 | 121.90 |
| 24 | YA | 1314 | C | C6-N1-C2 | -8.26 | 117.00 | 120.30 |
| 24 | YA | 828 | U | N1-C2-O2 | 8.23 | 128.56 | 122.80 |
| 24 | RA | 1407 | C | C6-N1-C2 | -8.22 | 117.01 | 120.30 |
| 24 | RA | 1931 | U | N3-C2-O2 | -8.21 | 116.45 | 122.20 |
| 24 | YA | 2726 | U | N3-C2-O2 | -8.21 | 116.45 | 122.20 |
| 24 | YA | 435 | C | N1-C2-O2 | 8.20 | 123.82 | 118.90 |
| 24 | YA | 1407 | C | C2-N1-C1' | 8.20 | 127.82 | 118.80 |
| 1 | QA | 1504 | G | C8-N9-C1' | -8.17 | 116.38 | 127.00 |
| 1 | XA | 1158 | C | C2-N1-C1' | 8.16 | 127.78 | 118.80 |
| 24 | RA | 1313 | U | N1-C2-O2 | 8.16 | 128.51 | 122.80 |
| 1 | QA | 1066 | C | N1-C2-O2 | 8.15 | 123.79 | 118.90 |
| 1 | QA | 328 | C | C6-N1-C2 | -8.12 | 117.05 | 120.30 |
| 1 | QA | 328 | C | C2-N1-C1' | 8.10 | 127.71 | 118.80 |
| 1 | QA | 1158 | C | C2-N1-C1' | 8.10 | 127.71 | 118.80 |
| 1 | QA | 1504 | G | C4-N9-C1' | 8.07 | 136.99 | 126.50 |
| 25 | RB | 31 | C | C2-N1-C1' | 8.00 | 127.60 | 118.80 |
| 24 | RA | 1519 | G | C8-N9-C1' | -7.99 | 116.61 | 127.00 |
| 1 | XA | 1158 | C | C6-N1-C2 | -7.97 | 117.11 | 120.30 |
| 24 | RA | 856 | C | C5-C6-N1 | 7.96 | 124.98 | 121.00 |
| 1 | QA | 754 | C | C2-N1-C1' | 7.93 | 127.53 | 118.80 |
| 24 | RA | 1417 | C | C5-C6-N1 | 7.92 | 124.96 | 121.00 |
| 24 | YA | 41 | C | C6-N1-C2 | -7.90 | 117.14 | 120.30 |
| 24 | RA | 1314 | C | C6-N1-C2 | -7.87 | 117.15 | 120.30 |
| 24 | YA | 749 | C | N1-C2-O2 | 7.86 | 123.61 | 118.90 |
| 24 | RA | 1519 | G | C4-N9-C1' | 7.84 | 136.70 | 126.50 |
| 24 | RA | 537 | C | C5-C6-N1 | 7.82 | 124.91 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 24 | YA | 1406 | U | C5-C6-N1 | 7.80 | 126.60 | 122.70 |
| 1 | QA | 110 | C | N1-C2-O2 | 7.79 | 123.57 | 118.90 |
| 24 | RA | 893 | C | N1-C2-O2 | 7.78 | 123.57 | 118.90 |
| 1 | QA | 1322 | C | N3-C2-O2 | -7.78 | 116.45 | 121.90 |
| 24 | RA | 828 | U | C2-N1-C1' | 7.76 | 127.02 | 117.70 |
| 24 | RA | 613 | U | N1-C2-O2 | 7.75 | 128.23 | 122.80 |
| 24 | YA | 1956 | U | N1-C2-O2 | 7.75 | 128.23 | 122.80 |
| 24 | YA | 860 | U | N1-C2-O2 | 7.74 | 128.22 | 122.80 |
| 23 | QX | 21 | G | C2'-C3'-O3' | 7.72 | 126.49 | 109.50 |
| 1 | XA | 747 | C | N1-C2-O2 | 7.69 | 123.51 | 118.90 |
| 1 | XA | 186(F) | C | N3-C2-O2 | -7.68 | 116.52 | 121.90 |
| 42 | YX | 66 | LEU | CA-CB-CG | 7.66 | 132.92 | 115.30 |
| 1 | QA | 1028(A) | C | N1-C2-O2 | 7.65 | 123.49 | 118.90 |
| 24 | YA | 1915 | U | N1-C2-O2 | 7.64 | 128.15 | 122.80 |
| 1 | QA | 307 | C | N1-C2-O2 | 7.60 | 123.46 | 118.90 |
| 24 | YA | 1658 | C | C5-C6-N1 | 7.60 | 124.80 | 121.00 |
| 24 | RA | 1535 | U | N1-C2-O2 | 7.59 | 128.12 | 122.80 |
| 24 | RA | 2666 | C | N3-C2-O2 | -7.59 | 116.59 | 121.90 |
| 24 | YA | 828 | U | N3-C2-O2 | -7.59 | 116.89 | 122.20 |
| 24 | RA | 1640 | C | C6-N1-C2 | -7.58 | 117.27 | 120.30 |
| 1 | QA | 1322 | C | C6-N1-C2 | -7.58 | 117.27 | 120.30 |
| 24 | YA | 1506 | C | C6-N1-C2 | -7.58 | 117.27 | 120.30 |
| 24 | YA | 2814 | C | N1-C2-O2 | 7.57 | 123.44 | 118.90 |
| 1 | XA | 110 | C | N1-C2-O2 | 7.57 | 123.44 | 118.90 |
| 1 | XA | 960 | U | N1-C2-O2 | 7.57 | 128.09 | 122.80 |
| 24 | RA | 537 | C | C6-N1-C2 | -7.54 | 117.28 | 120.30 |
| 25 | YB | 37 | C | N3-C2-O2 | -7.54 | 116.62 | 121.90 |
| 24 | RA | 1474 | C | C6-N1-C2 | -7.52 | 117.29 | 120.30 |
| 24 | YA | 2712(A) | A | C8-N9-C4 | -7.52 | 102.79 | 105.80 |
| 24 | RA | 607 | U | N1-C2-O2 | 7.49 | 128.04 | 122.80 |
| 24 | RA | 2063 | C | N1-C2-O2 | 7.49 | 123.39 | 118.90 |
| 1 | XA | 747 | C | N3-C2-O2 | -7.49 | 116.66 | 121.90 |
| 1 | XA | 135 | C | N3-C2-O2 | -7.48 | 116.66 | 121.90 |
| 24 | RA | 435 | C | N1-C2-O2 | 7.48 | 123.39 | 118.90 |
| 1 | XA | 1260 | C | N3-C2-O2 | -7.47 | 116.67 | 121.90 |
| 1 | QA | 1301 | U | C2-N1-C1' | 7.46 | 126.66 | 117.70 |
| 1 | XA | 135 | C | N1-C2-O2 | 7.46 | 123.38 | 118.90 |
| 24 | RA | 867 | C | N1-C2-O2 | 7.44 | 123.36 | 118.90 |
| 1 | XA | 979 | C | N3-C2-O2 | -7.44 | 116.69 | 121.90 |
| 24 | RA | 1407 | C | C2-N1-C1' | 7.43 | 126.98 | 118.80 |
| 24 | YA | 1658 | C | C6-N1-C2 | -7.43 | 117.33 | 120.30 |
| 24 | RA | 1005 | C | N1-C2-O2 | 7.43 | 123.36 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24 | RA | 2726 | U | N1-C2-O2 | 7.41 | 127.98 | 122.80 |
| 24 | RA | 546 | C | C6-N1-C2 | -7.40 | 117.34 | 120.30 |
| 1 | XA | 1260 | C | N1-C2-O2 | 7.37 | 123.32 | 118.90 |
| 24 | RA | 846 | C | N3-C2-O2 | -7.37 | 116.74 | 121.90 |
| 24 | RA | 1968 | G | O4'-C1'-N9 | 7.36 | 114.09 | 108.20 |
| 24 | YA | 867 | C | N1-C2-O2 | 7.35 | 123.31 | 118.90 |
| 1 | XA | 307 | C | N1-C2-O2 | 7.34 | 123.31 | 118.90 |
| 24 | YA | 1686 | C | C6-N1-C2 | -7.34 | 117.36 | 120.30 |
| 24 | YA | 556 | G | C6-C5-N7 | -7.33 | 126.00 | 130.40 |
| 24 | RA | 679 | C | C6-N1-C2 | -7.32 | 117.37 | 120.30 |
| 24 | RA | 613 | U | N3-C2-O2 | -7.32 | 117.08 | 122.20 |
| 24 | RA | 1640 | C | N3-C2-O2 | -7.32 | 116.78 | 121.90 |
| 24 | YA | 2063 | C | N1-C2-O2 | 7.31 | 123.28 | 118.90 |
| 24 | YA | 2726 | U | N1-C2-O2 | 7.29 | 127.90 | 122.80 |
| 24 | YA | 537 | C | C5-C6-N1 | 7.29 | 124.64 | 121.00 |
| 1 | QA | 1260 | C | C6-N1-C2 | -7.29 | 117.39 | 120.30 |
| 24 | YA | 2739 | U | N3-C2-O2 | -7.28 | 117.11 | 122.20 |
| 24 | RA | 2394 | C | N1-C2-O2 | 7.28 | 123.27 | 118.90 |
| 24 | YA | 385 | C | C6-N1-C2 | -7.28 | 117.39 | 120.30 |
| 14 | QN | 44 | LEU | CA-CB-CG | 7.25 | 131.98 | 115.30 |
| 1 | XA | 449 | C | N1-C2-O2 | 7.25 | 123.25 | 118.90 |
| 24 | RA | 846 | C | N1-C2-O2 | 7.24 | 123.24 | 118.90 |
| 24 | YA | 1670 | C | C6-N1-C1' | -7.22 | 112.13 | 120.80 |
| 24 | RA | 2726 | U | N3-C2-O2 | -7.22 | 117.14 | 122.20 |
| 24 | YA | 1417 | C | C5-C6-N1 | 7.22 | 124.61 | 121.00 |
| 24 | RA | 456 | C | N1-C2-O2 | 7.20 | 123.22 | 118.90 |
| 24 | RA | 1774 | C | C6-N1-C2 | -7.20 | 117.42 | 120.30 |
| 24 | RA | 1899 | G | N3-C4-N9 | -7.20 | 121.68 | 126.00 |
| 24 | YA | 1411 | C | C6-N1-C2 | -7.19 | 117.42 | 120.30 |
| 25 | YB | 31 | C | N3-C2-O2 | -7.19 | 116.86 | 121.90 |
| 24 | YA | 2701 | C | C6-N1-C2 | -7.19 | 117.42 | 120.30 |
| 22 | QV | 1 | C | C6-N1-C2 | -7.19 | 117.42 | 120.30 |
| 24 | RA | 1097 | U | N3-C2-O2 | -7.18 | 117.17 | 122.20 |
| 24 | RA | 607 | U | N3-C2-O2 | -7.18 | 117.17 | 122.20 |
| 22 | QV | 68 | U | N1-C2-O2 | 7.17 | 127.82 | 122.80 |
| 24 | RA | 546 | C | C2-N1-C1' | 7.16 | 126.67 | 118.80 |
| 24 | RA | 1956 | U | N1-C2-O2 | 7.15 | 127.81 | 122.80 |
| 1 | XA | 1452 | C | N1-C2-O2 | 7.14 | 123.18 | 118.90 |
| 1 | QA | 252 | U | N1-C2-O2 | 7.13 | 127.79 | 122.80 |
| 24 | YA | 2065 | C | C5-C6-N1 | 7.12 | 124.56 | 121.00 |
| 1 | QA | 328 | C | C5-C6-N1 | 7.12 | 124.56 | 121.00 |
| 1 | QA | 1228 | C | C6-N1-C2 | -7.10 | 117.46 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 24 | RA | 2321 | G | N3-C4-C5 | -7.08 | 125.06 | 128.60 |
| 1 | QA | 252 | U | N3-C2-O2 | -7.08 | 117.24 | 122.20 |
| 24 | YA | 753 | C | C6-N1-C2 | -7.07 | 117.47 | 120.30 |
| 1 | QA | 346 | G | N3-C4-C5 | -7.07 | 125.07 | 128.60 |
| 1 | XA | 618 | C | C6-N1-C2 | -7.06 | 117.47 | 120.30 |
| 24 | YA | 2065 | C | C6-N1-C2 | -7.06 | 117.47 | 120.30 |
| 24 | RA | 1097 | U | N1-C2-O2 | 7.06 | 127.74 | 122.80 |
| 24 | RA | 1474 | C | C5-C6-N1 | 7.05 | 124.53 | 121.00 |
| 24 | RA | 2847 | U | N1-C2-O2 | 7.05 | 127.73 | 122.80 |
| 38 | RT | 99 | LEU | CA-CB-CG | 7.05 | 131.51 | 115.30 |
| 1 | XA | 328 | C | C6-N1-C2 | -7.04 | 117.48 | 120.30 |
| 24 | RA | 1882 | C | C6-N1-C2 | -7.03 | 117.49 | 120.30 |
| 1 | XA | 1301 | U | N3-C2-O2 | -7.03 | 117.28 | 122.20 |
| 24 | YA | 435 | C | N3-C2-O2 | -7.02 | 116.98 | 121.90 |
| 24 | RA | 1313 | U | C2-N1-C1' | 7.01 | 126.11 | 117.70 |
| 24 | YA | 2321 | G | N3-C4-C5 | -7.01 | 125.09 | 128.60 |
| 24 | YA | 1950 | G | C4-N9-C1' | 7.00 | 135.61 | 126.50 |
| 25 | RB | 27 | C | N1-C2-O2 | 7.00 | 123.10 | 118.90 |
| 1 | QA | 789 | U | N3-C2-O2 | -7.00 | 117.30 | 122.20 |
| 1 | XA | 827 | U | N3-C2-O2 | -7.00 | 117.30 | 122.20 |
| 1 | XA | 1347 | G | C4-N9-C1' | -6.99 | 117.41 | 126.50 |
| 38 | YT | 99 | LEU | CA-CB-CG | 6.98 | 131.36 | 115.30 |
| 24 | RA | 2752 | C | N1-C2-O2 | 6.98 | 123.09 | 118.90 |
| 24 | RA | 2063 | C | N3-C2-O2 | -6.98 | 117.02 | 121.90 |
| 24 | RA | 2559 | C | N1-C2-O2 | 6.97 | 123.08 | 118.90 |
| 24 | YA | 2591 | C | C6-N1-C2 | -6.96 | 117.51 | 120.30 |
| 1 | XA | 346 | G | N3-C4-N9 | 6.96 | 130.18 | 126.00 |
| 24 | YA | 2394 | C | N1-C2-O2 | 6.96 | 123.08 | 118.90 |
| 24 | RA | 1742 | C | C6-N1-C2 | -6.96 | 117.52 | 120.30 |
| 25 | YB | 27 | C | N1-C2-O2 | 6.95 | 123.07 | 118.90 |
| 24 | YA | 915 | C | C6-N1-C2 | -6.94 | 117.52 | 120.30 |
| 24 | YA | 1064 | C | C6-N1-C2 | -6.93 | 117.53 | 120.30 |
| 24 | YA | 1534 | G | N3-C4-N9 | 6.92 | 130.15 | 126.00 |
| 24 | RA | 2321 | G | C8-N9-C4 | -6.91 | 103.64 | 106.40 |
| 24 | RA | 1514 | U | N1-C2-O2 | 6.90 | 127.63 | 122.80 |
| 24 | RA | 1294 | U | N3-C2-O2 | -6.90 | 117.37 | 122.20 |
| 24 | RA | 867 | C | N3-C2-O2 | -6.89 | 117.08 | 121.90 |
| 24 | RA | 1417 | C | C6-N1-C2 | -6.89 | 117.55 | 120.30 |
| 1 | XA | 497 | U | N3-C2-O2 | -6.88 | 117.38 | 122.20 |
| 1 | XA | 449 | C | N3-C2-O2 | -6.88 | 117.08 | 121.90 |
| 1 | XA | 1301 | U | N1-C2-O2 | 6.88 | 127.62 | 122.80 |
| 24 | YA | 2712(A) | A | C5-N7-C8 | -6.88 | 100.46 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24 | YA | 67 | U | C5-C6-N1 | 6.88 | 126.14 | 122.70 |
| 24 | YA | 265 | A | O4'-C1'-N9 | 6.86 | 113.69 | 108.20 |
| 1 | QA | 754 | C | N1-C2-O2 | 6.85 | 123.01 | 118.90 |
| 24 | RA | 1882 | C | C2-N1-C1' | 6.85 | 126.34 | 118.80 |
| 24 | RA | 1882 | C | C5-C6-N1 | 6.83 | 124.41 | 121.00 |
| 24 | RA | 1514 | U | N3-C2-O2 | -6.82 | 117.42 | 122.20 |
| 24 | YA | 537 | C | C6-N1-C2 | -6.82 | 117.57 | 120.30 |
| 24 | YA | 1506 | C | N1-C2-O2 | 6.79 | 122.98 | 118.90 |
| 22 | XV | 1 | C | C6-N1-C2 | -6.79 | 117.59 | 120.30 |
| 1 | XA | 529 | G | C5-C6-O6 | -6.78 | 124.53 | 128.60 |
| 22 | QV | 68 | U | N3-C2-O2 | -6.78 | 117.45 | 122.20 |
| 24 | RA | 2063 | C | C6-N1-C2 | -6.78 | 117.59 | 120.30 |
| 24 | YA | 867 | C | N3-C2-O2 | -6.78 | 117.15 | 121.90 |
| 1 | XA | 1260 | C | C6-N1-C2 | -6.77 | 117.59 | 120.30 |
| 24 | YA | 9 | U | N1-C2-O2 | 6.77 | 127.54 | 122.80 |
| 24 | RA | 635 | C | C6-N1-C2 | -6.75 | 117.60 | 120.30 |
| 24 | RA | 1914 | C | N3-C2-O2 | -6.75 | 117.18 | 121.90 |
| 1 | QA | 749 | C | N3-C2-O2 | -6.74 | 117.18 | 121.90 |
| 1 | XA | 1347 | G | C8-N9-C1' | 6.74 | 135.76 | 127.00 |
| 1 | XA | 135 | C | C6-N1-C2 | -6.73 | 117.61 | 120.30 |
| 24 | RA | 1509 | C | C2-N1-C1' | 6.72 | 126.19 | 118.80 |
| 24 | RA | 1535 | U | N3-C2-O2 | -6.71 | 117.50 | 122.20 |
| 1 | XA | 1028 | C | C6-N1-C2 | -6.71 | 117.62 | 120.30 |
| 24 | RA | 234 | C | N1-C2-O2 | 6.69 | 122.91 | 118.90 |
| 24 | YA | 2808 | U | N3-C2-O2 | -6.69 | 117.52 | 122.20 |
| 24 | RA | 1135 | C | N1-C2-O2 | 6.68 | 122.91 | 118.90 |
| 24 | YA | 2739 | U | N1-C2-O2 | 6.67 | 127.47 | 122.80 |
| 24 | RA | 537 | C | N1-C2-O2 | 6.66 | 122.90 | 118.90 |
| 9 | QI | 111 | ARG | CG-CD-NE | -6.66 | 97.82 | 111.80 |
| 24 | RA | 2096 | U | N1-C2-O2 | 6.64 | 127.45 | 122.80 |
| 25 | RB | 30 | C | C6-N1-C2 | -6.64 | 117.64 | 120.30 |
| 1 | XA | 1109 | C | N1-C2-O2 | 6.63 | 122.88 | 118.90 |
| 1 | XA | 330 | C | N3-C2-O2 | -6.63 | 117.26 | 121.90 |
| 24 | YA | 445 | C | C6-N1-C2 | -6.63 | 117.65 | 120.30 |
| 1 | XA | 754 | C | C2-N1-C1' | 6.62 | 126.09 | 118.80 |
| 1 | XA | 960 | U | N3-C2-O2 | -6.62 | 117.56 | 122.20 |
| 24 | YA | 1005 | C | N1-C2-O2 | 6.62 | 122.87 | 118.90 |
| 24 | YA | 2559 | C | C6-N1-C2 | -6.62 | 117.65 | 120.30 |
| 1 | XA | 346 | G | N3-C4-C5 | -6.62 | 125.29 | 128.60 |
| 24 | YA | 1407 | C | N1-C2-O2 | 6.62 | 122.87 | 118.90 |
| 22 | XV | 76 | C | C6-N1-C2 | -6.61 | 117.65 | 120.30 |
| 24 | YA | 9 | U | N3-C2-O2 | -6.61 | 117.57 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 24 | YA | 1506 | C | C5-C6-N1 | 6.61 | 124.31 | 121.00 |
| 24 | RA | 1835 | G | N3-C4-N9 | 6.61 | 129.97 | 126.00 |
| 1 | QA | 1066 | C | C2-N1-C1' | 6.60 | 126.06 | 118.80 |
| 1 | XA | 1109 | C | N3-C2-O2 | -6.60 | 117.28 | 121.90 |
| 24 | RA | 1686 | C | C6-N1-C2 | -6.59 | 117.66 | 120.30 |
| 24 | YA | 41 | C | C5-C6-N1 | 6.59 | 124.30 | 121.00 |
| 1 | QA | 1066 | C | C5-C6-N1 | 6.58 | 124.29 | 121.00 |
| 24 | YA | 2063 | C | N3-C2-O2 | -6.58 | 117.30 | 121.90 |
| 24 | YA | 1915 | U | N3-C2-O2 | -6.58 | 117.60 | 122.20 |
| 25 | YB | 31 | C | C6-N1-C2 | -6.58 | 117.67 | 120.30 |
| 1 | XA | 328 | C | C2-N1-C1' | 6.57 | 126.03 | 118.80 |
| 24 | YA | 1914 | C | N3-C2-O2 | -6.57 | 117.30 | 121.90 |
| 24 | YA | 1314 | C | C5-C6-N1 | 6.57 | 124.28 | 121.00 |
| 1 | QA | 169 | C | N1-C2-O2 | 6.56 | 122.84 | 118.90 |
| 24 | YA | 930 | U | N1-C2-O2 | 6.56 | 127.39 | 122.80 |
| 24 | YA | 2468 | G | C4-N9-C1' | 6.56 | 135.03 | 126.50 |
| 24 | YA | 12 | U | N1-C2-O2 | 6.56 | 127.39 | 122.80 |
| 24 | RA | 1835 | G | N3-C4-C5 | -6.56 | 125.32 | 128.60 |
| 24 | RA | 2096 | U | N3-C2-O2 | -6.55 | 117.61 | 122.20 |
| 24 | YA | 2343 | C | N3-C2-O2 | -6.55 | 117.31 | 121.90 |
| 24 | RA | 373 | U | C2-N1-C1' | 6.55 | 125.56 | 117.70 |
| 24 | YA | 1580 | A | C4-N9-C1' | 6.54 | 138.08 | 126.30 |
| 24 | YA | 243 | U | C5-C6-N1 | 6.54 | 125.97 | 122.70 |
| 24 | RA | 373 | U | C5-C6-N1 | 6.53 | 125.97 | 122.70 |
| 24 | YA | 1411 | C | C5-C6-N1 | 6.53 | 124.26 | 121.00 |
| 24 | RA | 2808 | U | N1-C2-O2 | 6.52 | 127.37 | 122.80 |
| 24 | YA | 1534 | G | N3-C4-C5 | -6.52 | 125.34 | 128.60 |
| 24 | RA | 1406 | U | N1-C2-O2 | 6.52 | 127.36 | 122.80 |
| 24 | YA | 828 | U | C5-C6-N1 | 6.51 | 125.96 | 122.70 |
| 25 | RB | 31 | C | C6-N1-C2 | -6.51 | 117.70 | 120.30 |
| 24 | YA | 2868 | A | C5-N7-C8 | -6.50 | 100.65 | 103.90 |
| 24 | RA | 2210 | G | N3-C4-N9 | 6.50 | 129.90 | 126.00 |
| 24 | RA | 2868 | A | C8-N9-C4 | -6.49 | 103.20 | 105.80 |
| 24 | RA | 2847 | U | N3-C2-O2 | -6.49 | 117.66 | 122.20 |
| 24 | YA | 141 | A | N7-C8-N9 | 6.49 | 117.04 | 113.80 |
| 24 | RA | 749 | C | N1-C2-O2 | 6.48 | 122.79 | 118.90 |
| 24 | YA | 1332 | G | C6-C5-N7 | -6.48 | 126.51 | 130.40 |
| 24 | YA | 373 | U | N3-C2-O2 | -6.47 | 117.67 | 122.20 |
| 24 | RA | 1920 | C | C5-C6-N1 | 6.47 | 124.23 | 121.00 |
| 24 | RA | 2666 | C | C6-N1-C2 | -6.47 | 117.71 | 120.30 |
| 1 | XA | 358 | U | P-O3'-C3' | 6.46 | 127.45 | 119.70 |
| 24 | YA | 1644 | C | N3-C2-O2 | -6.45 | 117.38 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 24 | RA | 2648 | C | C5-C6-N1 | 6.45 | 124.22 | 121.00 |
| 1 | XA | 449 | C | C6-N1-C2 | -6.45 | 117.72 | 120.30 |
| 24 | RA | 2720 | U | N3-C2-O2 | -6.44 | 117.69 | 122.20 |
| 24 | YA | 120 | U | C2-N1-C1' | 6.44 | 125.43 | 117.70 |
| 24 | RA | 2210 | G | N3-C4-C5 | -6.43 | 125.38 | 128.60 |
| 24 | YA | 1462 | C | N1-C2-O2 | 6.43 | 122.76 | 118.90 |
| 1 | QA | 1158 | C | C5-C6-N1 | 6.43 | 124.22 | 121.00 |
| 24 | YA | 1411 | C | N1-C2-O2 | 6.43 | 122.76 | 118.90 |
| 24 | RA | 546 | C | C5-C6-N1 | 6.42 | 124.21 | 121.00 |
| 24 | YA | 1332 | G | C4-N9-C1' | 6.42 | 134.85 | 126.50 |
| 1 | QA | 1344 | C | C6-N1-C2 | -6.42 | 117.73 | 120.30 |
| 24 | RA | 2188 | C | C6-N1-C2 | -6.41 | 117.73 | 120.30 |
| 1 | XA | 1158 | C | C5-C6-N1 | 6.41 | 124.21 | 121.00 |
| 1 | QA | 1109 | C | N1-C2-O2 | 6.41 | 122.75 | 118.90 |
| 24 | YA | 269 | U | N3-C2-O2 | -6.41 | 117.71 | 122.20 |
| 24 | RA | 2394 | C | N3-C2-O2 | -6.40 | 117.42 | 121.90 |
| 1 | QA | 1028(A) | C | N3-C2-O2 | -6.40 | 117.42 | 121.90 |
| 24 | RA | 1506 | C | N1-C2-O2 | 6.39 | 122.73 | 118.90 |
| 25 | RB | 37 | C | N1-C2-O2 | 6.39 | 122.73 | 118.90 |
| 24 | YA | 2321 | G | C8-N9-C4 | -6.38 | 103.85 | 106.40 |
| 24 | YA | 859 | G | P-O3'-C3' | 6.38 | 127.36 | 119.70 |
| 24 | RA | 2161 | C | N1-C2-O2 | 6.38 | 122.73 | 118.90 |
| 1 | XA | 497 | U | N1-C2-O2 | 6.38 | 127.27 | 122.80 |
| 24 | RA | 1005 | C | N3-C2-O2 | -6.38 | 117.44 | 121.90 |
| 24 | RA | 1314 | C | C5-C6-N1 | 6.38 | 124.19 | 121.00 |
| 24 | RA | 1658 | C | C6-N1-C2 | -6.37 | 117.75 | 120.30 |
| 1 | QA | 1066 | C | C6-N1-C2 | -6.36 | 117.75 | 120.30 |
| 24 | YA | 510 | C | C2-N1-C1' | 6.36 | 125.80 | 118.80 |
| 24 | YA | 1580 | A | C8-N9-C1' | -6.36 | 116.26 | 127.70 |
| 24 | YA | 2874 | C | N1-C2-O2 | 6.35 | 122.71 | 118.90 |
| 24 | YA | 2480 | C | N3-C2-O2 | -6.35 | 117.45 | 121.90 |
| 24 | YA | 537 | C | N1-C2-O2 | 6.33 | 122.70 | 118.90 |
| 24 | YA | 1686 | C | N1-C2-O2 | 6.33 | 122.70 | 118.90 |
| 24 | YA | 1678 | G | N7-C8-N9 | 6.33 | 116.26 | 113.10 |
| 24 | YA | 2096 | U | N3-C2-O2 | -6.33 | 117.77 | 122.20 |
| 24 | RA | 1406 | U | N3-C2-O2 | -6.32 | 117.78 | 122.20 |
| 24 | YA | 1314 | C | N1-C2-O2 | 6.32 | 122.69 | 118.90 |
| 24 | RA | 915 | C | C6-N1-C2 | -6.32 | 117.77 | 120.30 |
| 1 | XA | 307 | C | N3-C2-O2 | -6.32 | 117.48 | 121.90 |
| 24 | YA | 2808 | U | N1-C2-O2 | 6.31 | 127.21 | 122.80 |
| 24 | YA | 556 | G | N3-C4-N9 | 6.30 | 129.78 | 126.00 |
| 24 | YA | 1159 | U | C6-N1-C1' | -6.30 | 112.37 | 121.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25 | RB | 37 | C | N3-C2-O2 | -6.30 | 117.49 | 121.90 |
| 24 | YA | 1411 | C | C2-N1-C1' | 6.29 | 125.72 | 118.80 |
| 24 | RA | 729 | G | C4-N9-C1' | 6.29 | 134.68 | 126.50 |
| 22 | QV | 76 | C | C6-N1-C2 | -6.29 | 117.78 | 120.30 |
| 24 | YA | 753 | C | C5-C6-N1 | 6.29 | 124.14 | 121.00 |
| 24 | RA | 456 | C | N3-C2-O2 | -6.28 | 117.50 | 121.90 |
| 14 | XN | 44 | LEU | CA-CB-CG | 6.28 | 129.74 | 115.30 |
| 24 | YA | 797 | C | C6-N1-C2 | -6.28 | 117.79 | 120.30 |
| 24 | YA | 783 | A | C5-N7-C8 | -6.26 | 100.77 | 103.90 |
| 24 | YA | 1234 | U | N3-C2-O2 | -6.26 | 117.82 | 122.20 |
| 24 | RA | 2808 | U | N3-C2-O2 | -6.26 | 117.82 | 122.20 |
| 24 | YA | 846 | C | C2'-C3'-O3' | 6.25 | 123.71 | 113.70 |
| 24 | YA | 556 | G | N7-C8-N9 | 6.25 | 116.22 | 113.10 |
| 24 | RA | 2591 | C | C6-N1-C2 | -6.25 | 117.80 | 120.30 |
| 24 | RA | 1332 | G | C6-C5-N7 | -6.24 | 126.66 | 130.40 |
| 24 | RA | 1640 | C | C5-C6-N1 | 6.24 | 124.12 | 121.00 |
| 24 | RA | 2739 | U | N3-C2-O2 | -6.24 | 117.84 | 122.20 |
| 24 | YA | 1640 | C | C6-N1-C2 | -6.23 | 117.81 | 120.30 |
| 24 | YA | 1005 | C | C2-N1-C1' | 6.23 | 125.65 | 118.80 |
| 1 | QA | 749 | C | N1-C2-O2 | 6.23 | 122.64 | 118.90 |
| 1 | XA | 749 | C | C6-N1-C2 | -6.23 | 117.81 | 120.30 |
| 24 | RA | 1372 | U | N1-C2-O2 | 6.23 | 127.16 | 122.80 |
| 24 | YA | 234 | C | N1-C2-O2 | 6.22 | 122.63 | 118.90 |
| 24 | YA | 893 | C | N1-C2-O2 | 6.22 | 122.63 | 118.90 |
| 1 | XA | 110 | C | N3-C2-O2 | -6.22 | 117.55 | 121.90 |
| 25 | YB | 30 | C | C6-N1-C2 | -6.22 | 117.81 | 120.30 |
| 24 | RA | 817 | C | C6-N1-C2 | -6.21 | 117.81 | 120.30 |
| 24 | RA | 1644 | C | C6-N1-C2 | -6.21 | 117.81 | 120.30 |
| 1 | XA | 1452 | C | N3-C2-O2 | -6.21 | 117.55 | 121.90 |
| 24 | RA | 2752 | C | N3-C2-O2 | -6.21 | 117.55 | 121.90 |
| 1 | QA | 1301 | U | C5-C6-N1 | 6.21 | 125.81 | 122.70 |
| 24 | RA | 1064 | C | C6-N1-C2 | -6.20 | 117.82 | 120.30 |
| 24 | YA | 2688 | U | N3-C2-O2 | -6.20 | 117.86 | 122.20 |
| 24 | YA | 269 | U | N1-C2-O2 | 6.19 | 127.13 | 122.80 |
| 1 | XA | 1228 | C | C6-N1-C2 | -6.19 | 117.83 | 120.30 |
| 24 | RA | 1528 | A | N7-C8-N9 | 6.18 | 116.89 | 113.80 |
| 24 | YA | 783 | A | N7-C8-N9 | 6.18 | 116.89 | 113.80 |
| 24 | YA | 2501 | C | C2-N1-C1' | -6.18 | 112.00 | 118.80 |
| 1 | QA | 110 | C | N3-C2-O2 | -6.17 | 117.58 | 121.90 |
| 24 | YA | 2210 | G | N3-C4-C5 | -6.16 | 125.52 | 128.60 |
| 24 | RA | 1914 | C | C2-N1-C1' | 6.16 | 125.57 | 118.80 |
| 24 | YA | 2578 | G | N1-C6-O6 | -6.15 | 116.21 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 24 | RA | 923 | C | C5-C6-N1 | 6.15 | 124.07 | 121.00 |
| 24 | YA | 758 | C | N3-C2-O2 | -6.14 | 117.60 | 121.90 |
| 24 | RA | 904 | C | N1-C2-O2 | 6.14 | 122.58 | 118.90 |
| 1 | XA | 1140 | C | C6-N1-C2 | -6.14 | 117.84 | 120.30 |
| 1 | XA | 1161 | C | N1-C2-O2 | 6.14 | 122.59 | 118.90 |
| 24 | YA | 1013 | C | C6-N1-C2 | -6.14 | 117.85 | 120.30 |
| 24 | RA | 1407 | C | C5-C6-N1 | 6.13 | 124.07 | 121.00 |
| 24 | RA | 2559 | C | N3-C2-O2 | -6.13 | 117.61 | 121.90 |
| 25 | RB | 43 | C | N1-C2-O2 | 6.13 | 122.58 | 118.90 |
| 1 | XA | 1028(B) | C | C6-N1-C2 | -6.12 | 117.85 | 120.30 |
| 1 | QA | 346 | G | C2-N3-C4 | 6.12 | 114.96 | 111.90 |
| 24 | RA | 1513 | C | N1-C2-O2 | 6.11 | 122.57 | 118.90 |
| 24 | YA | 2210 | G | N3-C4-N9 | 6.11 | 129.67 | 126.00 |
| 38 | YT | 99 | LEU | CB-CG-CD1 | -6.11 | 100.61 | 111.00 |
| 24 | RA | 893 | C | N3-C2-O2 | -6.11 | 117.63 | 121.90 |
| 1 | QA | 307 | C | N3-C2-O2 | -6.10 | 117.63 | 121.90 |
| 24 | YA | 1644 | C | N1-C2-O2 | 6.10 | 122.56 | 118.90 |
| 1 | XA | 252 | U | C5-C6-N1 | 6.10 | 125.75 | 122.70 |
| 24 | RA | 1902 | C | N1-C2-O2 | 6.09 | 122.56 | 118.90 |
| 24 | RA | 1505 | C | N1-C2-O2 | 6.09 | 122.56 | 118.90 |
| 24 | YA | 2307 | G | C4-N9-C1' | 6.09 | 134.42 | 126.50 |
| 24 | RA | 2688 | U | N3-C2-O2 | -6.09 | 117.94 | 122.20 |
| 24 | RA | 640 | C | C5-C6-N1 | 6.09 | 124.04 | 121.00 |
| 24 | YA | 1882 | C | C6-N1-C2 | -6.08 | 117.87 | 120.30 |
| 24 | YA | 2041 | U | C5-C6-N1 | 6.08 | 125.74 | 122.70 |
| 1 | QA | 1118 | C | N1-C2-O2 | 6.07 | 122.54 | 118.90 |
| 24 | YA | 857 | C | C6-N1-C2 | -6.07 | 117.87 | 120.30 |
| 1 | QA | 1279 | A | N7-C8-N9 | 6.07 | 116.83 | 113.80 |
| 24 | RA | 976 | C | C6-N1-C2 | -6.07 | 117.87 | 120.30 |
| 24 | YA | 783 | A | C8-N9-C4 | -6.07 | 103.37 | 105.80 |
| 24 | RA | 1833 | U | N3-C2-O2 | -6.07 | 117.95 | 122.20 |
| 24 | RA | 1406 | U | C5-C6-N1 | 6.06 | 125.73 | 122.70 |
| 24 | YA | 2584 | U | N3-C2-O2 | -6.06 | 117.96 | 122.20 |
| 24 | YA | 1640 | C | N1-C2-O2 | 6.06 | 122.54 | 118.90 |
| 24 | YA | 1430 | C | C6-N1-C2 | -6.05 | 117.88 | 120.30 |
| 24 | RA | 120 | U | C2-N1-C1' | 6.05 | 124.96 | 117.70 |
| 24 | RA | 1658 | C | C5-C6-N1 | 6.04 | 124.02 | 121.00 |
| 24 | RA | 2043 | C | C5-C6-N1 | 6.04 | 124.02 | 121.00 |
| 1 | XA | 328 | C | C5-C6-N1 | 6.04 | 124.02 | 121.00 |
| 24 | RA | 856 | C | N1-C2-O2 | 6.04 | 122.52 | 118.90 |
| 1 | QA | 1147 | C | N3-C2-O2 | -6.04 | 117.67 | 121.90 |
| 24 | YA | 141 | A | C5-N7-C8 | -6.04 | 100.88 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 24 | YA | 1430 | C | C5-C6-N1 | 6.03 | 124.02 | 121.00 |
| 24 | YA | 12 | U | N3-C2-O2 | -6.03 | 117.98 | 122.20 |
| 24 | RA | 2868 | A | N7-C8-N9 | 6.01 | 116.81 | 113.80 |
| 1 | QA | 1066 | C | N3-C2-O2 | -6.01 | 117.69 | 121.90 |
| 24 | YA | 1961 | C | N3-C2-O2 | -6.01 | 117.69 | 121.90 |
| 24 | RA | 1407 | C | N1-C2-O2 | 6.01 | 122.50 | 118.90 |
| 25 | RB | 27 | C | N3-C2-O2 | -6.01 | 117.69 | 121.90 |
| 24 | YA | 672 | C | C6-N1-C2 | -6.01 | 117.90 | 120.30 |
| 24 | YA | 2210 | G | C4-N9-C1' | 6.01 | 134.31 | 126.50 |
| 24 | YA | 2712 | U | N3-C2-O2 | -6.01 | 118.00 | 122.20 |
| 24 | YA | 1604 | C | C6-N1-C2 | -6.00 | 117.90 | 120.30 |
| 1 | QA | 1395 | C | N1-C2-O2 | 6.00 | 122.50 | 118.90 |
| 24 | YA | 856 | C | N3-C2-O2 | -6.00 | 117.70 | 121.90 |
| 22 | XV | 68 | U | N1-C2-O2 | 6.00 | 127.00 | 122.80 |
| 24 | YA | 640 | C | C6-N1-C2 | -6.00 | 117.90 | 120.30 |
| 24 | YA | 1675 | C | C6-N1-C2 | -5.99 | 117.90 | 120.30 |
| 24 | YA | 2096 | U | N1-C2-O2 | 5.99 | 126.99 | 122.80 |
| 22 | XV | 68 | U | N3-C2-O2 | -5.99 | 118.01 | 122.20 |
| 24 | RA | 1332 | G | C4-N9-C1' | 5.98 | 134.28 | 126.50 |
| 24 | YA | 930 | U | N3-C2-O2 | -5.97 | 118.02 | 122.20 |
| 1 | QA | 1260 | C | N3-C2-O2 | -5.97 | 117.72 | 121.90 |
| 24 | RA | 2420 | C | C5-C6-N1 | 5.97 | 123.98 | 121.00 |
| 1 | XA | 826 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 24 | YA | 1644 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 24 | YA | 1437 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 1 | XA | 1028 | C | N1-C2-O2 | 5.96 | 122.48 | 118.90 |
| 24 | RA | 1686 | C | N1-C2-O2 | 5.96 | 122.48 | 118.90 |
| 25 | YB | 27 | C | N3-C2-O2 | -5.96 | 117.73 | 121.90 |
| 24 | RA | 1437 | C | C6-N1-C2 | -5.96 | 117.92 | 120.30 |
| 1 | QA | 455 | C | N1-C2-O2 | 5.95 | 122.47 | 118.90 |
| 1 | XA | 330 | C | C6-N1-C2 | -5.95 | 117.92 | 120.30 |
| 24 | YA | 860 | U | C6-N1-C1' | 5.94 | 129.52 | 121.20 |
| 24 | YA | 1406 | U | C6-N1-C2 | -5.94 | 117.44 | 121.00 |
| 24 | RA | 1644 | C | N1-C2-O2 | 5.94 | 122.46 | 118.90 |
| 24 | YA | 1306 | C | C5-C6-N1 | 5.94 | 123.97 | 121.00 |
| 24 | YA | 1313 | U | C6-N1-C1' | -5.94 | 112.89 | 121.20 |
| 24 | RA | 2043 | C | C6-N1-C2 | -5.93 | 117.93 | 120.30 |
| 24 | RA | 2683 | C | N1-C2-O2 | 5.93 | 122.46 | 118.90 |
| 24 | YA | 1882 | C | C2-N1-C1' | 5.93 | 125.32 | 118.80 |
| 24 | YA | 749 | C | N3-C2-O2 | -5.93 | 117.75 | 121.90 |
| 22 | QV | 1 | C | C5-C6-N1 | 5.92 | 123.96 | 121.00 |
| 1 | QA | 1109 | C | N3-C2-O2 | -5.92 | 117.75 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 24 | YA | 654(T) | C | N1-C2-O2 | 5.92 | 122.45 | 118.90 |
| 24 | YA | 2559 | C | N1-C2-O2 | 5.92 | 122.45 | 118.90 |
| 24 | RA | 537 | C | C2-N1-C1' | 5.92 | 125.31 | 118.80 |
| 1 | QA | 754 | C | C6-N1-C1' | -5.91 | 113.70 | 120.80 |
| 24 | RA | 265 | A | O4'-C1'-N9 | 5.91 | 112.93 | 108.20 |
| 24 | YA | 459 | U | N3-C2-O2 | -5.91 | 118.06 | 122.20 |
| 24 | YA | 2043 | C | C6-N1-C2 | -5.91 | 117.94 | 120.30 |
| 24 | YA | 2155 | G | N3-C4-N9 | 5.90 | 129.54 | 126.00 |
| 24 | RA | 1528 | A | C8-N9-C4 | -5.90 | 103.44 | 105.80 |
| 24 | RA | 2473 | U | N1-C2-O2 | 5.90 | 126.93 | 122.80 |
| 24 | YA | 856 | C | N1-C2-O2 | 5.90 | 122.44 | 118.90 |
| 24 | RA | 2739 | U | N1-C2-O2 | 5.90 | 126.93 | 122.80 |
| 24 | RA | 435 | C | N3-C2-O2 | -5.89 | 117.77 | 121.90 |
| 1 | QA | 1147 | C | N1-C2-O2 | 5.89 | 122.44 | 118.90 |
| 24 | RA | 2720 | U | N1-C2-O2 | 5.89 | 126.92 | 122.80 |
| 38 | RT | 105 | LEU | CA-CB-CG | 5.89 | 128.84 | 115.30 |
| 24 | YA | 234 | C | N3-C2-O2 | -5.88 | 117.78 | 121.90 |
| 24 | RA | 2874 | C | N1-C2-O2 | 5.88 | 122.43 | 118.90 |
| 1 | XA | 1140 | C | C2-N1-C1' | 5.88 | 125.27 | 118.80 |
| 24 | YA | 640 | C | C5-C6-N1 | 5.88 | 123.94 | 121.00 |
| 24 | YA | 1686 | C | C5-C6-N1 | 5.87 | 123.94 | 121.00 |
| 24 | RA | 1065 | U | N3-C2-O2 | -5.87 | 118.09 | 122.20 |
| 24 | RA | 2473 | U | N3-C2-O2 | -5.87 | 118.09 | 122.20 |
| 1 | QA | 1381 | U | N1-C2-O2 | 5.87 | 126.91 | 122.80 |
| 24 | YA | 797 | C | C5-C6-N1 | 5.87 | 123.93 | 121.00 |
| 24 | RA | 456 | C | C6-N1-C2 | -5.85 | 117.96 | 120.30 |
| 1 | XA | 789 | U | N3-C2-O2 | -5.85 | 118.11 | 122.20 |
| 1 | QA | 90 | C | N1-C2-O2 | 5.85 | 122.41 | 118.90 |
| 1 | XA | 827 | U | C6-N1-C2 | -5.85 | 117.49 | 121.00 |
| 24 | RA | 2825 | C | C6-N1-C2 | -5.84 | 117.96 | 120.30 |
| 24 | YA | 192 | C | N3-C2-O2 | -5.84 | 117.81 | 121.90 |
| 24 | YA | 1950 | G | C8-N9-C1' | -5.84 | 119.41 | 127.00 |
| 24 | RA | 1417 | C | N1-C2-O2 | 5.84 | 122.40 | 118.90 |
| 1 | QA | 449 | C | N1-C2-O2 | 5.84 | 122.40 | 118.90 |
| 24 | RA | 2726 | U | C2-N1-C1' | 5.83 | 124.70 | 117.70 |
| 24 | RA | 730 | C | P-O3'-C3' | 5.83 | 126.69 | 119.70 |
| 1 | XA | 1395 | C | N1-C2-O2 | 5.83 | 122.40 | 118.90 |
| 24 | YA | 1095 | A | C2-N3-C4 | 5.83 | 113.51 | 110.60 |
| 24 | YA | 2702 | U | C5-C6-N1 | 5.82 | 125.61 | 122.70 |
| 25 | YB | 37 | C | C6-N1-C2 | -5.82 | 117.97 | 120.30 |
| 24 | RA | 776 | G | N3-C4-C5 | -5.82 | 125.69 | 128.60 |
| 24 | YA | 1881 | C | C6-N1-C2 | -5.82 | 117.97 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 24 | RA | 273(F) | C | C6-N1-C2 | -5.82 | 117.97 | 120.30 |
| 24 | YA | 1599 | C | C6-N1-C2 | -5.82 | 117.97 | 120.30 |
| 1 | XA | 169 | C | N1-C2-O2 | 5.81 | 122.39 | 118.90 |
| 24 | YA | 2825 | C | C6-N1-C2 | -5.81 | 117.97 | 120.30 |
| 25 | RB | 22 | U | N3-C2-O2 | -5.81 | 118.13 | 122.20 |
| 1 | QA | 1026 | G | N3-C4-N9 | 5.81 | 129.49 | 126.00 |
| 24 | RA | 976 | C | N1-C2-O2 | 5.80 | 122.38 | 118.90 |
| 24 | RA | 1314 | C | N1-C2-O2 | 5.80 | 122.38 | 118.90 |
| 24 | RA | 2210 | G | C4-N9-C1' | 5.80 | 134.04 | 126.50 |
| 1 | XA | 979 | C | C6-N1-C2 | -5.79 | 117.98 | 120.30 |
| 24 | RA | 1686 | C | C5-C6-N1 | 5.79 | 123.90 | 121.00 |
| 1 | XA | 455 | C | N1-C2-O2 | 5.79 | 122.38 | 118.90 |
| 1 | QA | 449 | C | C2-N1-C1' | 5.79 | 125.17 | 118.80 |
| 24 | RA | 309 | G | OP1-P-OP2 | -5.79 | 110.92 | 119.60 |
| 1 | XA | 749 | C | N3-C2-O2 | -5.79 | 117.85 | 121.90 |
| 1 | XA | 1028 | C | N3-C2-O2 | -5.79 | 117.85 | 121.90 |
| 24 | YA | 1332 | G | C8-N9-C1' | -5.78 | 119.48 | 127.00 |
| 24 | YA | 1343 | G | N3-C4-C5 | -5.78 | 125.71 | 128.60 |
| 24 | YA | 1407 | C | N3-C2-O2 | -5.78 | 117.85 | 121.90 |
| 24 | YA | 1535 | U | C2-N1-C1' | 5.78 | 124.64 | 117.70 |
| 24 | YA | 2320 | A | C2-N3-C4 | 5.78 | 113.49 | 110.60 |
| 24 | RA | 120 | U | C6-N1-C2 | -5.78 | 117.53 | 121.00 |
| 1 | XA | 528 | C | N1-C2-O2 | 5.78 | 122.37 | 118.90 |
| 25 | RB | 44 | G | C4-N9-C1' | -5.77 | 119.00 | 126.50 |
| 24 | RA | 595 | C | C5-C6-N1 | 5.77 | 123.89 | 121.00 |
| 24 | RA | 2825 | C | N3-C2-O2 | -5.77 | 117.86 | 121.90 |
| 1 | QA | 754 | C | N3-C2-O2 | -5.76 | 117.86 | 121.90 |
| 22 | XV | 35 | C | N1-C2-O2 | 5.76 | 122.36 | 118.90 |
| 1 | XA | 738 | C | C5-C6-N1 | 5.76 | 123.88 | 121.00 |
| 1 | QA | 435 | C | C5-C6-N1 | 5.76 | 123.88 | 121.00 |
| 24 | RA | 1474 | C | N1-C2-O2 | 5.76 | 122.35 | 118.90 |
| 24 | YA | 692 | C | C6-N1-C2 | -5.75 | 118.00 | 120.30 |
| 24 | YA | 1979 | C | C6-N1-C2 | -5.75 | 118.00 | 120.30 |
| 24 | YA | 1533 | C | C5-C6-N1 | 5.75 | 123.88 | 121.00 |
| 24 | RA | 856 | C | N3-C2-O2 | -5.75 | 117.88 | 121.90 |
| 24 | YA | 2394 | C | N3-C2-O2 | -5.75 | 117.88 | 121.90 |
| 1 | QA | 697 | U | N3-C2-O2 | -5.74 | 118.18 | 122.20 |
| 24 | RA | 2501 | C | C2-N1-C1' | -5.74 | 112.48 | 118.80 |
| 24 | YA | 2559 | C | N3-C2-O2 | -5.74 | 117.88 | 121.90 |
| 1 | XA | 618 | C | N3-C2-O2 | -5.74 | 117.88 | 121.90 |
| 24 | YA | 1588 | C | C6-N1-C2 | -5.74 | 118.01 | 120.30 |
| 25 | RB | 22 | U | N1-C2-O2 | 5.73 | 126.81 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | QA | 1020 | U | N1-C2-O2 | 5.73 | 126.81 | 122.80 |
| 24 | YA | 1474 | C | C6-N1-C2 | -5.73 | 118.01 | 120.30 |
| 24 | RA | 2556 | C | N1-C2-O2 | 5.73 | 122.33 | 118.90 |
| 1 | QA | 697 | U | N1-C2-O2 | 5.72 | 126.81 | 122.80 |
| 25 | RB | 31 | C | C5-C6-N1 | 5.72 | 123.86 | 121.00 |
| 24 | RA | 595 | C | C6-N1-C2 | -5.72 | 118.01 | 120.30 |
| 1 | XA | 35 | G | C6-C5-N7 | -5.71 | 126.97 | 130.40 |
| 24 | YA | 231 | C | C6-N1-C2 | -5.71 | 118.01 | 120.30 |
| 24 | RA | 1462 | C | N3-C2-O2 | -5.71 | 117.90 | 121.90 |
| 24 | RA | 1899 | G | N3-C2-N2 | -5.71 | 115.90 | 119.90 |
| 1 | XA | 530 | G | N3-C4-N9 | 5.71 | 129.43 | 126.00 |
| 24 | YA | 2726 | U | C2-N1-C1' | 5.71 | 124.55 | 117.70 |
| 25 | YB | 31 | C | C6-N1-C1' | -5.71 | 113.95 | 120.80 |
| 1 | XA | 1362(A) | C | N3-C2-O2 | -5.70 | 117.91 | 121.90 |
| 24 | YA | 1920 | C | C5-C6-N1 | 5.70 | 123.85 | 121.00 |
| 1 | QA | 652 | U | N3-C2-O2 | -5.70 | 118.21 | 122.20 |
| 24 | RA | 1267 | U | N3-C2-O2 | -5.69 | 118.22 | 122.20 |
| 1 | XA | 749 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 24 | YA | 2712 | U | C2-N1-C1' | 5.68 | 124.52 | 117.70 |
| 24 | YA | 2787 | C | C6-N1-C2 | -5.68 | 118.03 | 120.30 |
| 24 | YA | 1781 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 9 | XI | 2 | GLU | N-CA-C | -5.68 | 95.66 | 111.00 |
| 1 | QA | 37 | U | N3-C2-O2 | -5.68 | 118.23 | 122.20 |
| 1 | QA | 1065 | U | P-O3'-C3' | 5.68 | 126.51 | 119.70 |
| 24 | RA | 758 | C | N3-C2-O2 | -5.68 | 117.93 | 121.90 |
| 1 | XA | 1395 | C | N3-C2-O2 | -5.67 | 117.93 | 121.90 |
| 24 | YA | 650 | C | C6-N1-C2 | -5.67 | 118.03 | 120.30 |
| 44 | YZ | 5 | LEU | CA-CB-CG | 5.67 | 128.35 | 115.30 |
| 22 | XV | 35 | C | C6-N1-C2 | -5.67 | 118.03 | 120.30 |
| 24 | YA | 1961 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 24 | YA | 529 | A | C8-N9-C4 | -5.67 | 103.53 | 105.80 |
| 24 | YA | 1202 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 25 | YB | 31 | C | C5-C6-N1 | 5.67 | 123.84 | 121.00 |
| 24 | YA | 2416 | C | C6-N1-C2 | -5.67 | 118.03 | 120.30 |
| 1 | QA | 1186 | G | N3-C4-N9 | 5.67 | 129.40 | 126.00 |
| 24 | YA | 1666 | G | N1-C6-O6 | -5.67 | 116.50 | 119.90 |
| 24 | YA | 2100 | G | N3-C4-C5 | -5.66 | 125.77 | 128.60 |
| 24 | YA | 2889 | C | N1-C2-O2 | 5.66 | 122.30 | 118.90 |
| 24 | RA | 1882 | C | N1-C2-O2 | 5.66 | 122.30 | 118.90 |
| 24 | YA | 2155 | G | N3-C4-C5 | -5.66 | 125.77 | 128.60 |
| 1 | QA | 346 | G | N3-C4-N9 | 5.66 | 129.39 | 126.00 |
| 24 | RA | 2468 | G | C4-N9-C1' | 5.66 | 133.85 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24 | YA | 2179 | C | C6-N1-C2 | -5.65 | 118.04 | 120.30 |
| 24 | YA | 2342 | C | N3-C2-O2 | -5.65 | 117.94 | 121.90 |
| 24 | RA | 308 | G | O4'-C1'-N9 | 5.65 | 112.72 | 108.20 |
| 24 | YA | 120 | U | C6-N1-C2 | -5.65 | 117.61 | 121.00 |
| 1 | XA | 442 | C | N1-C2-O2 | 5.64 | 122.29 | 118.90 |
| 24 | YA | 2179 | C | N1-C2-O2 | 5.64 | 122.29 | 118.90 |
| 25 | RB | 44 | G | C8-N9-C1' | 5.64 | 134.33 | 127.00 |
| 24 | YA | 1774 | C | C6-N1-C2 | -5.64 | 118.04 | 120.30 |
| 24 | YA | 556 | G | C4-C5-N7 | 5.64 | 113.06 | 110.80 |
| 24 | RA | 2248 | C | C6-N1-C2 | -5.63 | 118.05 | 120.30 |
| 24 | YA | 755 | C | C6-N1-C2 | -5.63 | 118.05 | 120.30 |
| 24 | YA | 1462 | C | N3-C2-O2 | -5.63 | 117.96 | 121.90 |
| 24 | RA | 1920 | C | C6-N1-C2 | -5.62 | 118.05 | 120.30 |
| 24 | RA | 2321 | G | C4-N9-C1' | 5.62 | 133.81 | 126.50 |
| 24 | YA | 1332 | G | N3-C4-N9 | 5.62 | 129.37 | 126.00 |
| 24 | RA | 1742 | C | N1-C2-O2 | 5.62 | 122.27 | 118.90 |
| 24 | YA | 857 | C | C5-C6-N1 | 5.62 | 123.81 | 121.00 |
| 24 | YA | 2814 | C | C6-N1-C2 | -5.62 | 118.05 | 120.30 |
| 26 | YD | 34 | VAL | C-N-CA | 5.62 | 135.74 | 121.70 |
| 25 | RB | 43 | C | N3-C2-O2 | -5.61 | 117.97 | 121.90 |
| 24 | YA | 2073 | C | C6-N1-C2 | -5.60 | 118.06 | 120.30 |
| 24 | RA | 867 | C | C6-N1-C2 | -5.59 | 118.06 | 120.30 |
| 24 | YA | 654 | A | C2-N3-C4 | 5.59 | 113.40 | 110.60 |
| 24 | YA | 1256 | G | N3-C4-C5 | -5.59 | 125.80 | 128.60 |
| 24 | RA | 234 | C | N3-C2-O2 | -5.59 | 117.99 | 121.90 |
| 24 | YA | 459 | U | N1-C2-O2 | 5.59 | 126.71 | 122.80 |
| 24 | YA | 1313 | U | C6-N1-C2 | -5.59 | 117.65 | 121.00 |
| 24 | YA | 2683 | C | N1-C2-O2 | 5.59 | 122.25 | 118.90 |
| 24 | RA | 749 | C | N3-C2-O2 | -5.59 | 117.99 | 121.90 |
| 1 | QA | 960 | U | N1-C2-O2 | 5.58 | 126.71 | 122.80 |
| 24 | RA | 1544 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 24 | RA | 1742 | C | C5-C6-N1 | 5.58 | 123.79 | 121.00 |
| 1 | XA | 618 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 1 | QA | 1395 | C | N3-C2-O2 | -5.58 | 118.00 | 121.90 |
| 24 | RA | 1947 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 24 | RA | 2066 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 25 | RB | 37 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 24 | YA | 1417 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 24 | YA | 2667 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |
| 24 | YA | 2794 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 24 | RA | 285 | C | N1-C2-O2 | 5.56 | 122.24 | 118.90 |
| 24 | RA | 912 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 24 | YA | 2785 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 24 | RA | 1135 | C | N3-C2-O2 | -5.56 | 118.01 | 121.90 |
| 24 | YA | 1157 | G | C4-N9-C1' | 5.56 | 133.73 | 126.50 |
| 24 | RA | 1510 | A | C2-N3-C4 | 5.56 | 113.38 | 110.60 |
| 24 | RA | 1644 | C | N3-C2-O2 | -5.56 | 118.01 | 121.90 |
| 24 | RA | 1979 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 24 | YA | 1882 | C | N1-C2-O2 | 5.56 | 122.23 | 118.90 |
| 31 | YI | 35 | LEU | CA-CB-CG | 5.56 | 128.08 | 115.30 |
| 24 | RA | 1980 | G | C4-N9-C1' | 5.55 | 133.72 | 126.50 |
| 24 | YA | 1257 | C | C6-N1-C2 | -5.55 | 118.08 | 120.30 |
| 24 | YA | 1534 | G | C2-N3-C4 | 5.55 | 114.68 | 111.90 |
| 2 | QB | 158 | LEU | CA-CB-CG | 5.55 | 128.07 | 115.30 |
| 24 | RA | 669 | G | N3-C4-C5 | -5.55 | 125.82 | 128.60 |
| 24 | YA | 1882 | C | C5-C6-N1 | 5.55 | 123.78 | 121.00 |
| 24 | YA | 2490 | G | C4-N9-C1' | 5.55 | 133.72 | 126.50 |
| 24 | RA | 1549 | C | N1-C2-O2 | 5.55 | 122.23 | 118.90 |
| 1 | XA | 186(F) | C | N1-C2-O2 | 5.54 | 122.23 | 118.90 |
| 24 | YA | 1064 | C | C5-C6-N1 | 5.54 | 123.77 | 121.00 |
| 1 | QA | 1118 | C | N3-C2-O2 | -5.54 | 118.02 | 121.90 |
| 24 | YA | 2343 | C | N1-C2-O2 | 5.54 | 122.22 | 118.90 |
| 13 | XM | 66 | LEU | C-N-CA | 5.54 | 135.54 | 121.70 |
| 24 | RA | 708 | C | N1-C2-O2 | 5.53 | 122.22 | 118.90 |
| 24 | YA | 99 | U | OP2-P-O3' | 5.53 | 117.37 | 105.20 |
| 24 | YA | 1267 | U | N3-C2-O2 | -5.53 | 118.33 | 122.20 |
| 25 | RB | 27 | C | C6-N1-C2 | -5.53 | 118.09 | 120.30 |
| 1 | XA | 738 | C | C6-N1-C2 | -5.53 | 118.09 | 120.30 |
| 8 | QH | 112 | LEU | CA-CB-CG | 5.52 | 128.01 | 115.30 |
| 24 | RA | 155 | C | N1-C2-O2 | 5.52 | 122.21 | 118.90 |
| 24 | YA | 1077 | A | C2-N3-C4 | 5.52 | 113.36 | 110.60 |
| 24 | RA | 1656 | C | C6-N1-C2 | -5.52 | 118.09 | 120.30 |
| 1 | QA | 1020 | U | N3-C2-O2 | -5.51 | 118.34 | 122.20 |
| 24 | RA | 2666 | C | C5-C6-N1 | 5.50 | 123.75 | 121.00 |
| 22 | XV | 76 | C | C5-C6-N1 | 5.50 | 123.75 | 121.00 |
| 24 | RA | 965 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 24 | RA | 1407 | C | N3-C2-O2 | -5.50 | 118.05 | 121.90 |
| 24 | RA | 2006 | C | C5-C6-N1 | 5.50 | 123.75 | 121.00 |
| 24 | YA | 848 | G | N3-C4-N9 | 5.50 | 129.30 | 126.00 |
| 24 | YA | 2342 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 1 | QA | 91 | C | N1-C2-O2 | 5.49 | 122.20 | 118.90 |
| 24 | RA | 373 | U | C6-N1-C2 | -5.49 | 117.70 | 121.00 |
| 1 | XA | 1290 | G | N3-C4-N9 | 5.49 | 129.30 | 126.00 |
| 24 | YA | 1598 | C | C6-N1-C2 | -5.49 | 118.10 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 24 | YA | 2244 | U | C5-C4-O4 | -5.49 | 122.60 | 125.90 |
| 24 | RA | 797 | C | C6-N1-C2 | -5.49 | 118.10 | 120.30 |
| 24 | YA | 2031 | A | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 24 | YA | 2089 | U | N3-C2-O2 | -5.49 | 118.36 | 122.20 |
| 1 | XA | 221 | C | C6-N1-C2 | -5.49 | 118.10 | 120.30 |
| 1 | QA | 328 | C | P-O3'-C3' | 5.49 | 126.28 | 119.70 |
| 24 | RA | 2578 | G | N1-C6-O6 | -5.49 | 116.61 | 119.90 |
| 1 | XA | 1404 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 24 | YA | 1830 | C | C5-C6-N1 | 5.47 | 123.74 | 121.00 |
| 24 | RA | 1961 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 24 | RA | 2874 | C | C6-N1-C2 | -5.47 | 118.11 | 120.30 |
| 24 | RA | 915 | C | N1-C2-O2 | 5.46 | 122.18 | 118.90 |
| 24 | RA | 1505 | C | C5-C6-N1 | 5.46 | 123.73 | 121.00 |
| 24 | YA | 1370 | C | C6-N1-C2 | -5.46 | 118.11 | 120.30 |
| 24 | YA | 828 | U | C6-N1-C1' | -5.46 | 113.55 | 121.20 |
| 24 | YA | 1306 | C | N1-C2-O2 | 5.46 | 122.18 | 118.90 |
| 24 | RA | 731 | C | C2-N1-C1' | 5.46 | 124.80 | 118.80 |
| 1 | QA | 58 | C | C6-N1-C2 | -5.46 | 118.12 | 120.30 |
| 24 | RA | 1372 | U | C2-N3-C4 | 5.46 | 130.27 | 127.00 |
| 24 | RA | 1505 | C | C6-N1-C2 | -5.46 | 118.12 | 120.30 |
| 24 | YA | 944 | G | C4-N9-C1' | 5.46 | 133.59 | 126.50 |
| 24 | RA | 459 | U | N3-C2-O2 | -5.45 | 118.38 | 122.20 |
| 24 | YA | 1905 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 24 | RA | 1675 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 1 | XA | 449 | C | C2-N1-C1' | 5.45 | 124.80 | 118.80 |
| 24 | YA | 208 | C | C6-N1-C2 | -5.45 | 118.12 | 120.30 |
| 24 | RA | 2688 | U | N1-C2-O2 | 5.44 | 126.61 | 122.80 |
| 24 | YA | 1157 | G | C8-N9-C1' | -5.44 | 119.92 | 127.00 |
| 24 | YA | 679 | C | C6-N1-C2 | -5.44 | 118.12 | 120.30 |
| 24 | RA | 776 | G | N3-C4-N9 | 5.44 | 129.26 | 126.00 |
| 24 | RA | 2248 | C | C5-C6-N1 | 5.44 | 123.72 | 121.00 |
| 24 | YA | 1675 | C | N1-C2-O2 | 5.43 | 122.16 | 118.90 |
| 1 | QA | 563 | A | C4-N9-C1' | 5.43 | 136.08 | 126.30 |
| 1 | XA | 1404 | C | N3-C2-O2 | -5.43 | 118.10 | 121.90 |
| 24 | YA | 721 | C | C6-N1-C2 | -5.43 | 118.13 | 120.30 |
| 24 | YA | 974(A) | C | N1-C2-O2 | 5.43 | 122.16 | 118.90 |
| 24 | RA | 2006 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 24 | YA | 2468 | G | C8-N9-C1' | -5.42 | 119.95 | 127.00 |
| 24 | RA | 2692 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 1 | QA | 749 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 24 | RA | 2870 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 24 | YA | 2648 | C | C5-C6-N1 | 5.42 | 123.71 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | XA | 54 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 24 | YA | 641 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 24 | YA | 1598 | C | N3-C2-O2 | -5.42 | 118.11 | 121.90 |
| 1 | XA | 960 | U | C2-N1-C1' | 5.41 | 124.20 | 117.70 |
| 24 | RA | 828 | U | C5-C6-N1 | 5.41 | 125.40 | 122.70 |
| 24 | YA | 1678 | G | C8-N9-C4 | -5.41 | 104.24 | 106.40 |
| 24 | YA | 2128 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 26 | RD | 34 | VAL | C-N-CA | 5.40 | 135.21 | 121.70 |
| 24 | RA | 1053 | C | C6-N1-C2 | -5.40 | 118.14 | 120.30 |
| 24 | RA | 1533 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 24 | RA | 2683 | C | N3-C2-O2 | -5.40 | 118.12 | 121.90 |
| 24 | RA | 1506 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 1 | XA | 1113 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 24 | RA | 1881 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 1 | XA | 1514 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 24 | RA | 912 | C | N1-C2-O2 | 5.39 | 122.13 | 118.90 |
| 24 | YA | 1507 | A | C2-N3-C4 | 5.39 | 113.29 | 110.60 |
| 24 | RA | 93 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 24 | RA | 420 | C | C6-N1-C2 | -5.39 | 118.15 | 120.30 |
| 24 | RA | 1046 | A | C2-N3-C4 | 5.39 | 113.29 | 110.60 |
| 1 | XA | 530 | G | N3-C4-C5 | -5.39 | 125.91 | 128.60 |
| 24 | RA | 1909 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 1 | XA | 529 | G | C4-C5-N7 | 5.38 | 112.95 | 110.80 |
| 24 | YA | 654(T) | C | N3-C2-O2 | -5.38 | 118.14 | 121.90 |
| 24 | YA | 2342 | C | N1-C2-O2 | 5.38 | 122.12 | 118.90 |
| 24 | YA | 384 | U | N3-C2-O2 | -5.37 | 118.44 | 122.20 |
| 1 | QA | 1028(A) | C | C6-N1-C2 | -5.37 | 118.15 | 120.30 |
| 24 | RA | 1433 | U | N1-C2-O2 | 5.37 | 126.56 | 122.80 |
| 1 | XA | 1439 | C | C6-N1-C2 | -5.37 | 118.15 | 120.30 |
| 1 | QA | 1381 | U | N3-C2-O2 | -5.36 | 118.44 | 122.20 |
| 1 | QA | 1263 | C | N1-C2-O2 | 5.36 | 122.12 | 118.90 |
| 19 | QS | 8 | GLY | N-CA-C | 5.36 | 126.50 | 113.10 |
| 1 | XA | 330 | C | C5-C6-N1 | 5.36 | 123.68 | 121.00 |
| 24 | YA | 1021 | A | C8-N9-C4 | -5.36 | 103.66 | 105.80 |
| 24 | RA | 2307 | G | C4-N9-C1' | 5.36 | 133.46 | 126.50 |
| 24 | YA | 267 | C | C6-N1-C2 | -5.35 | 118.16 | 120.30 |
| 24 | YA | 817 | C | C6-N1-C2 | -5.35 | 118.16 | 120.30 |
| 42 | RX | 66 | LEU | CA-CB-CG | 5.35 | 127.61 | 115.30 |
| 24 | YA | 1598 | C | N1-C2-O2 | 5.35 | 122.11 | 118.90 |
| 24 | RA | 2468 | G | O4'-C1'-N9 | 5.34 | 112.48 | 108.20 |
| 1 | XA | 328 | C | P-O3'-C3' | 5.34 | 126.11 | 119.70 |
| 24 | YA | 2681 | C | P-O3'-C3' | 5.34 | 126.11 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24 | YA | 1779 | U | C2-N1-C1' | 5.34 | 124.11 | 117.70 |
| 24 | RA | 436 | C | N3-C2-O2 | -5.34 | 118.16 | 121.90 |
| 1 | XA | 252 | U | C2-N1-C1' | 5.34 | 124.11 | 117.70 |
| 24 | YA | 1535 | U | C5-C6-N1 | 5.34 | 125.37 | 122.70 |
| 24 | RA | 2254 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 24 | YA | 1290 | C | C6-N1-C2 | -5.33 | 118.17 | 120.30 |
| 24 | RA | 1267 | U | N1-C2-O2 | 5.33 | 126.53 | 122.80 |
| 24 | YA | 1474 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 1 | QA | 449 | C | N3-C2-O2 | -5.33 | 118.17 | 121.90 |
| 24 | YA | 1881 | C | C5-C6-N1 | 5.33 | 123.66 | 121.00 |
| 1 | XA | 812 | C | P-O3'-C3' | 5.32 | 126.09 | 119.70 |
| 22 | XV | 1 | C | C5-C6-N1 | 5.32 | 123.66 | 121.00 |
| 24 | RA | 730 | C | C2'-C3'-O3' | 5.31 | 122.20 | 113.70 |
| 24 | YA | 1833 | U | N3-C2-O2 | -5.31 | 118.48 | 122.20 |
| 24 | YA | 18 | C | C6-N1-C2 | -5.31 | 118.18 | 120.30 |
| 1 | QA | 1452 | C | N1-C2-O2 | 5.31 | 122.08 | 118.90 |
| 24 | RA | 2065 | C | C5-C6-N1 | 5.31 | 123.65 | 121.00 |
| 24 | YA | 1544 | C | N1-C2-O2 | 5.31 | 122.08 | 118.90 |
| 24 | RA | 2814 | C | N3-C2-O2 | -5.30 | 118.19 | 121.90 |
| 1 | XA | 714 | G | C8-N9-C4 | -5.30 | 104.28 | 106.40 |
| 1 | XA | 1228 | C | C5-C6-N1 | 5.30 | 123.65 | 121.00 |
| 24 | RA | 1202 | C | N1-C2-O2 | 5.30 | 122.08 | 118.90 |
| 24 | YA | 2771 | C | C6-N1-C2 | -5.30 | 118.18 | 120.30 |
| 1 | QA | 397 | A | C2-N3-C4 | 5.30 | 113.25 | 110.60 |
| 24 | RA | 1947 | C | C6-N1-C2 | -5.30 | 118.18 | 120.30 |
| 24 | RA | 1947 | C | C5-C6-N1 | 5.30 | 123.65 | 121.00 |
| 24 | YA | 1005 | C | C6-N1-C2 | -5.30 | 118.18 | 120.30 |
| 24 | RA | 2101 | G | N7-C8-N9 | 5.30 | 115.75 | 113.10 |
| 25 | RB | 77 | U | N3-C2-O2 | -5.30 | 118.49 | 122.20 |
| 1 | QA | 1260 | C | N1-C2-O2 | 5.30 | 122.08 | 118.90 |
| 24 | YA | 2779 | U | N1-C2-O2 | 5.29 | 126.50 | 122.80 |
| 24 | RA | 201 | C | N3-C2-O2 | -5.28 | 118.20 | 121.90 |
| 24 | YA | 1669 | A | C2-N3-C4 | 5.28 | 113.24 | 110.60 |
| 1 | QA | 1121 | U | C5-C6-N1 | 5.28 | 125.34 | 122.70 |
| 24 | YA | 1892 | C | C6-N1-C2 | -5.28 | 118.19 | 120.30 |
| 24 | YA | 2584 | U | N1-C2-O2 | 5.28 | 126.50 | 122.80 |
| 24 | RA | 2856 | C | C6-N1-C2 | -5.28 | 118.19 | 120.30 |
| 24 | YA | 672 | C | C5-C6-N1 | 5.28 | 123.64 | 121.00 |
| 24 | RA | 1462 | C | N1-C2-O2 | 5.28 | 122.07 | 118.90 |
| 24 | RA | 417 | C | C5-C6-N1 | 5.28 | 123.64 | 121.00 |
| 24 | RA | 1372 | U | N3-C2-O2 | -5.28 | 118.51 | 122.20 |
| 25 | YB | 22 | U | N3-C2-O2 | -5.28 | 118.51 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24 | RA | 487 | C | N1-C2-O2 | 5.27 | 122.06 | 118.90 |
| 1 | XA | 1290 | G | N3-C4-C5 | -5.27 | 125.96 | 128.60 |
| 24 | RA | 1370 | C | C6-N1-C2 | -5.27 | 118.19 | 120.30 |
| 1 | QA | 56 | U | C5-C4-O4 | -5.27 | 122.74 | 125.90 |
| 24 | RA | 2556 | C | N3-C2-O2 | -5.27 | 118.21 | 121.90 |
| 24 | YA | 2712 | U | N1-C2-O2 | 5.27 | 126.49 | 122.80 |
| 24 | RA | 669 | G | N3-C4-N9 | 5.27 | 129.16 | 126.00 |
| 1 | XA | 58 | C | C5-C6-N1 | 5.26 | 123.63 | 121.00 |
| 24 | YA | 155 | C | N1-C2-O2 | 5.26 | 122.06 | 118.90 |
| 24 | YA | 976 | C | C6-N1-C2 | -5.26 | 118.19 | 120.30 |
| 1 | QA | 528 | C | C6-N1-C2 | -5.26 | 118.20 | 120.30 |
| 5 | QE | 91 | LEU | CA-CB-CG | 5.26 | 127.40 | 115.30 |
| 24 | RA | 2043 | C | N1-C2-O2 | 5.26 | 122.06 | 118.90 |
| 24 | RA | 1509 | C | C6-N1-C1' | -5.26 | 114.49 | 120.80 |
| 24 | RA | 2501 | C | C6-N1-C1' | 5.26 | 127.11 | 120.80 |
| 24 | YA | 1005 | C | N3-C2-O2 | -5.26 | 118.22 | 121.90 |
| 1 | QA | 960 | U | N3-C2-O2 | -5.25 | 118.52 | 122.20 |
| 1 | XA | 792 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 24 | RA | 1510 | A | N3-C4-N9 | 5.25 | 131.60 | 127.40 |
| 24 | YA | 1881 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 24 | RA | 729 | G | C8-N9-C1' | -5.25 | 120.18 | 127.00 |
| 1 | QA | 652 | U | N1-C2-O2 | 5.24 | 126.47 | 122.80 |
| 24 | RA | 1180 | C | N1-C2-O2 | 5.24 | 122.05 | 118.90 |
| 24 | YA | 2015 | A | N7-C8-N9 | 5.24 | 116.42 | 113.80 |
| 1 | QA | 1228 | C | C5-C6-N1 | 5.24 | 123.62 | 121.00 |
| 24 | RA | 269 | U | N3-C2-O2 | -5.24 | 118.53 | 122.20 |
| 24 | YA | 912 | C | N1-C2-O2 | 5.24 | 122.04 | 118.90 |
| 24 | YA | 1314 | C | N3-C2-O2 | -5.24 | 118.23 | 121.90 |
| 24 | RA | 1065 | U | N1-C2-O2 | 5.24 | 126.47 | 122.80 |
| 24 | RA | 1535 | U | C2-N1-C1' | 5.24 | 123.99 | 117.70 |
| 1 | QA | 1070 | U | N3-C2-O2 | -5.24 | 118.53 | 122.20 |
| 24 | YA | 99 | U | P-O3'-C3' | 5.24 | 125.98 | 119.70 |
| 24 | YA | 580 | C | C6-N1-C2 | -5.23 | 118.21 | 120.30 |
| 1 | QA | 943 | U | N3-C2-O2 | -5.23 | 118.54 | 122.20 |
| 24 | RA | 529 | A | C8-N9-C4 | -5.23 | 103.71 | 105.80 |
| 24 | YA | 1675 | C | N3-C2-O2 | -5.23 | 118.24 | 121.90 |
| 24 | YA | 2688 | U | C2-N1-C1' | 5.22 | 123.97 | 117.70 |
| 1 | QA | 419 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 9 | XI | 56 | LEU | CA-CB-CG | 5.22 | 127.31 | 115.30 |
| 24 | YA | 595 | C | C5-C6-N1 | 5.22 | 123.61 | 121.00 |
| 1 | XA | 137 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 24 | RA | 897 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 24 | RA | 898 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 24 | RA | 1332 | G | C8-N9-C1' | -5.21 | 120.22 | 127.00 |
| 1 | QA | 789 | U | N1-C2-O2 | 5.21 | 126.44 | 122.80 |
| 24 | YA | 1549 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 1 | XA | 943 | U | N3-C2-O2 | -5.21 | 118.56 | 122.20 |
| 24 | YA | 2724 | C | N3-C2-O2 | -5.21 | 118.26 | 121.90 |
| 24 | YA | 669 | G | N3-C4-C5 | -5.21 | 126.00 | 128.60 |
| 24 | YA | 2043 | C | C2-N1-C1' | 5.20 | 124.52 | 118.80 |
| 24 | YA | 2591 | C | C5-C6-N1 | 5.20 | 123.60 | 121.00 |
| 1 | XA | 1132 | C | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 1 | XA | 1347 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 24 | RA | 1915 | U | N1-C2-O2 | 5.20 | 126.44 | 122.80 |
| 24 | YA | 417 | C | C5-C6-N1 | 5.20 | 123.60 | 121.00 |
| 24 | YA | 1830 | C | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 24 | RA | 2460 | U | N3-C2-O2 | -5.19 | 118.56 | 122.20 |
| 24 | YA | 2450 | A | N7-C8-N9 | 5.19 | 116.40 | 113.80 |
| 24 | YA | 2683 | C | N3-C2-O2 | -5.19 | 118.27 | 121.90 |
| 1 | QA | 789 | U | C2-N1-C1' | 5.19 | 123.93 | 117.70 |
| 1 | QA | 923 | A | N7-C8-N9 | 5.19 | 116.39 | 113.80 |
| 24 | RA | 2073 | C | C6-N1-C2 | -5.19 | 118.22 | 120.30 |
| 24 | RA | 2442 | C | C6-N1-C2 | -5.19 | 118.22 | 120.30 |
| 26 | RD | 131 | LEU | CA-CB-CG | 5.19 | 127.23 | 115.30 |
| 1 | XA | 54 | C | N3-C2-O2 | -5.19 | 118.27 | 121.90 |
| 25 | RB | 8 | U | N1-C2-O2 | 5.18 | 126.43 | 122.80 |
| 24 | YA | 372 | G | C4-N9-C1' | -5.18 | 119.76 | 126.50 |
| 1 | QA | 169 | C | N3-C2-O2 | -5.18 | 118.27 | 121.90 |
| 24 | RA | 1915 | U | N3-C2-O2 | -5.18 | 118.57 | 122.20 |
| 24 | RA | 273(F) | C | C5-C6-N1 | 5.18 | 123.59 | 121.00 |
| 22 | XV | 35 | C | N3-C2-O2 | -5.18 | 118.28 | 121.90 |
| 24 | YA | 1234 | U | N1-C2-O2 | 5.18 | 126.42 | 122.80 |
| 24 | YA | 2874 | C | N3-C2-O2 | -5.18 | 118.28 | 121.90 |
| 24 | YA | 2248 | C | C6-N1-C2 | -5.18 | 118.23 | 120.30 |
| 24 | RA | 2403 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 24 | YA | 2724 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 24 | RA | 1675 | C | N3-C2-O2 | -5.17 | 118.28 | 121.90 |
| 24 | RA | 1502 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 24 | YA | 508 | G | N3-C4-C5 | -5.17 | 126.02 | 128.60 |
| 24 | RA | 1433 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 24 | RA | 1971 | A | C2-N3-C4 | 5.17 | 113.18 | 110.60 |
| 24 | YA | 923 | C | C5-C6-N1 | 5.17 | 123.58 | 121.00 |
| 24 | YA | 1551 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 24 | YA | 837 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | QA | 932 | C | N1-C2-O2 | 5.16 | 122.00 | 118.90 |
| 24 | RA | 2461 | C | N1-C2-O2 | 5.16 | 122.00 | 118.90 |
| 24 | RA | 2161 | C | N3-C2-O2 | -5.16 | 118.29 | 121.90 |
| 24 | RA | 2351 | G | C8-N9-C4 | -5.16 | 104.34 | 106.40 |
| 24 | YA | 1640 | C | C5-C6-N1 | 5.16 | 123.58 | 121.00 |
| 24 | RA | 436 | C | N1-C2-O2 | 5.15 | 121.99 | 118.90 |
| 25 | RB | 31 | C | C6-N1-C1' | -5.15 | 114.62 | 120.80 |
| 24 | YA | 1513 | C | C5-C6-N1 | 5.15 | 123.58 | 121.00 |
| 24 | YA | 2701 | C | C5-C6-N1 | 5.15 | 123.58 | 121.00 |
| 24 | RA | 1920 | C | N1-C2-O2 | 5.15 | 121.99 | 118.90 |
| 24 | RA | 923 | C | C6-N1-C2 | -5.15 | 118.24 | 120.30 |
| 24 | YA | 2626 | C | C6-N1-C2 | -5.15 | 118.24 | 120.30 |
| 24 | YA | 1604 | C | N3-C2-O2 | -5.15 | 118.30 | 121.90 |
| 24 | RA | 1810 | A | C8-N9-C4 | -5.14 | 103.74 | 105.80 |
| 24 | YA | 503 | A | P-O3'-C3' | 5.14 | 125.87 | 119.70 |
| 1 | XA | 699 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 24 | YA | 2752 | C | N1-C2-O2 | 5.14 | 121.99 | 118.90 |
| 1 | XA | 347 | G | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 24 | RA | 2626 | C | C6-N1-C2 | -5.14 | 118.25 | 120.30 |
| 24 | YA | 1306 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 1 | QA | 620 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 1 | QA | 1059 | C | C6-N1-C2 | -5.14 | 118.25 | 120.30 |
| 24 | RA | 343 | C | C6-N1-C2 | -5.14 | 118.25 | 120.30 |
| 1 | QA | 1279 | A | C8-N9-C4 | -5.14 | 103.75 | 105.80 |
| 22 | QV | 76 | C | C5-C6-N1 | 5.14 | 123.57 | 121.00 |
| 1 | XA | 620 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 24 | RA | 640 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 24 | YA | 2471 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 1 | QA | 1498 | U | P-O3'-C3' | 5.13 | 125.86 | 119.70 |
| 1 | QA | 266 | G | C5-C6-O6 | -5.13 | 125.52 | 128.60 |
| 24 | RA | 2626 | C | C5-C6-N1 | 5.13 | 123.56 | 121.00 |
| 24 | YA | 537 | C | C2-N1-C1' | 5.13 | 124.44 | 118.80 |
| 24 | RA | 1598 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 24 | RA | 1775 | U | C5-C4-O4 | -5.13 | 122.82 | 125.90 |
| 24 | YA | 1178 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 24 | RA | 308 | G | OP2-P-O3' | -5.13 | 93.92 | 105.20 |
| 24 | YA | 196 | A | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 24 | RA | 2211 | G | C4-N9-C1' | 5.12 | 133.16 | 126.50 |
| 1 | XA | 1225 | A | C2-N3-C4 | 5.11 | 113.16 | 110.60 |
| 24 | YA | 183 | C | N3-C2-O2 | -5.11 | 118.32 | 121.90 |
| 24 | YA | 1591 | G | N3-C4-N9 | 5.11 | 129.07 | 126.00 |
| 24 | RA | 2755 | C | C6-N1-C2 | -5.11 | 118.25 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24 | YA | 2015 | A | C8-N9-C4 | -5.11 | 103.75 | 105.80 |
| 24 | RA | 2889 | C | N1-C2-O2 | 5.11 | 121.97 | 118.90 |
| 1 | QA | 675 | A | N7-C8-N9 | 5.11 | 116.35 | 113.80 |
| 24 | RA | 976 | C | N3-C2-O2 | -5.11 | 118.33 | 121.90 |
| 24 | YA | 1293 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 24 | RA | 1314 | C | C2-N1-C1' | 5.11 | 124.42 | 118.80 |
| 24 | YA | 867 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 24 | YA | 595 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 1 | QA | 1500 | A | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 9 | QI | 53 | VAL | CA-CB-CG1 | 5.10 | 118.55 | 110.90 |
| 1 | XA | 1297 | C | P-O3'-C3' | 5.10 | 125.82 | 119.70 |
| 24 | YA | 1776 | G | N3-C4-N9 | 5.10 | 129.06 | 126.00 |
| 25 | YB | 70 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 24 | RA | 2646 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 24 | YA | 231 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 24 | YA | 2416 | C | C5-C6-N1 | 5.10 | 123.55 | 121.00 |
| 1 | QA | 522 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 24 | RA | 105 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 24 | RA | 634 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 25 | RB | 77 | U | N1-C2-O2 | 5.10 | 126.37 | 122.80 |
| 24 | YA | 143 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 24 | YA | 1343 | G | N3-C4-N9 | 5.10 | 129.06 | 126.00 |
| 1 | XA | 1498 | U | P-O3'-C3' | 5.10 | 125.81 | 119.70 |
| 24 | YA | 1640 | C | N3-C2-O2 | -5.09 | 118.33 | 121.90 |
| 24 | YA | 2794 | C | N1-C2-O2 | 5.09 | 121.96 | 118.90 |
| 1 | QA | 738 | C | C5-C6-N1 | 5.09 | 123.55 | 121.00 |
| 24 | RA | 404 | C | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 24 | YA | 2658 | C | N3-C2-O2 | -5.09 | 118.34 | 121.90 |
| 24 | RA | 459 | U | N1-C2-O2 | 5.09 | 126.36 | 122.80 |
| 24 | YA | 1679 | U | N1-C2-O2 | 5.09 | 126.36 | 122.80 |
| 24 | YA | 1894 | C | C6-N1-C2 | -5.09 | 118.27 | 120.30 |
| 1 | XA | 252 | U | N1-C2-O2 | 5.08 | 126.36 | 122.80 |
| 1 | QA | 54 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 24 | RA | 2137 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 24 | RA | 529 | A | C2-N3-C4 | 5.08 | 113.14 | 110.60 |
| 24 | YA | 2720 | U | N3-C2-O2 | -5.08 | 118.64 | 122.20 |
| 24 | YA | 234 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 25 | YB | 22 | U | N1-C2-O2 | 5.08 | 126.36 | 122.80 |
| 24 | RA | 1207 | C | C5-C6-N1 | 5.08 | 123.54 | 121.00 |
| 24 | RA | 2456 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 24 | YA | 1526 | G | C6-C5-N7 | -5.08 | 127.36 | 130.40 |
| 44 | YZ | 150 | LEU | CA-CB-CG | 5.08 | 126.97 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | QA | 169 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 1 | QA | 563 | A | C8-N9-C1' | -5.07 | 118.58 | 127.70 |
| 24 | YA | 2759 | G | N3-C4-N9 | 5.07 | 129.04 | 126.00 |
| 24 | RA | 248 | G | C6-C5-N7 | -5.07 | 127.36 | 130.40 |
| 24 | RA | 308 | G | OP1-P-O3' | 5.07 | 116.34 | 105.20 |
| 24 | YA | 67 | U | C6-N1-C2 | -5.07 | 117.96 | 121.00 |
| 26 | YD | 32 | SER | C-N-CA | 5.07 | 134.37 | 121.70 |
| 24 | RA | 1513 | C | N3-C2-O2 | -5.06 | 118.36 | 121.90 |
| 24 | RA | 1598 | C | N3-C2-O2 | -5.06 | 118.36 | 121.90 |
| 1 | QA | 528 | C | N1-C2-O2 | 5.06 | 121.94 | 118.90 |
| 24 | RA | 1370 | C | N1-C2-O2 | 5.06 | 121.94 | 118.90 |
| 24 | RA | 1902 | C | N3-C2-O2 | -5.06 | 118.36 | 121.90 |
| 1 | XA | 1140 | C | C5-C6-N1 | 5.06 | 123.53 | 121.00 |
| 24 | RA | 1686 | C | C2-N1-C1' | 5.05 | 124.36 | 118.80 |
| 24 | YA | 828 | U | C6-N1-C2 | -5.05 | 117.97 | 121.00 |
| 24 | YA | 893 | C | N3-C2-O2 | -5.05 | 118.36 | 121.90 |
| 1 | QA | 1303 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 24 | RA | 2043 | C | C2-N1-C1' | 5.05 | 124.35 | 118.80 |
| 24 | YA | 271(B) | G | P-O3'-C3' | 5.05 | 125.75 | 119.70 |
| 24 | YA | 413 | C | C6-N1-C2 | -5.05 | 118.28 | 120.30 |
| 24 | RA | 785 | G | C8-N9-C4 | -5.04 | 104.38 | 106.40 |
| 24 | RA | 2248 | C | N1-C2-O2 | 5.04 | 121.93 | 118.90 |
| 24 | YA | 755 | C | C5-C6-N1 | 5.04 | 123.52 | 121.00 |
| 1 | XA | 345 | C | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 1 | XA | 812 | C | OP2-P-O3' | 5.04 | 116.29 | 105.20 |
| 24 | YA | 2056 | G | N3-C4-N9 | 5.04 | 129.02 | 126.00 |
| 1 | QA | 252 | U | C2-N1-C1' | 5.04 | 123.75 | 117.70 |
| 24 | RA | 691 | C | C6-N1-C2 | -5.04 | 118.28 | 120.30 |
| 24 | RA | 1049 | C | C6-N1-C2 | -5.04 | 118.28 | 120.30 |
| 1 | XA | 618 | C | C5-C6-N1 | 5.04 | 123.52 | 121.00 |
| 9 | QI | 111 | ARG | NE-CZ-NH1 | 5.03 | 122.82 | 120.30 |
| 24 | RA | 2321 | G | N7-C8-N9 | 5.03 | 115.62 | 113.10 |
| 24 | RA | 2825 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 1 | XA | 993 | G | N3-C4-N9 | 5.03 | 129.02 | 126.00 |
| 24 | YA | 1830 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 24 | RA | 1487 | G | N3-C4-N9 | 5.03 | 129.02 | 126.00 |
| 1 | XA | 56 | U | N3-C4-O4 | 5.03 | 122.92 | 119.40 |
| 1 | XA | 1028 | C | C5-C6-N1 | 5.03 | 123.51 | 121.00 |
| 24 | RA | 641 | C | C5-C6-N1 | 5.03 | 123.51 | 121.00 |
| 24 | YA | 1135 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 24 | YA | 1686 | C | C2-N1-C1' | 5.02 | 124.33 | 118.80 |
| 1 | QA | 1439 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 24 | RA | 828 | U | C6-N1-C2 | -5.02 | 117.99 | 121.00 |
| 24 | RA | 1513 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 24 | YA | 114 | U | N3-C2-O2 | -5.02 | 118.68 | 122.20 |
| 24 | YA | 2307 | G | C8-N9-C1' | -5.02 | 120.47 | 127.00 |
| 24 | RA | 1864 | U | N3-C2-O2 | -5.02 | 118.69 | 122.20 |
| 1 | QA | 1378 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 24 | RA | 2233 | U | N3-C2-O2 | -5.02 | 118.69 | 122.20 |
| 24 | RA | 1644 | C | C5-C6-N1 | 5.02 | 123.51 | 121.00 |
| 24 | RA | 1899 | G | N9-C4-C5 | 5.02 | 107.41 | 105.40 |
| 24 | YA | 856 | C | C2-N1-C1' | 5.02 | 124.32 | 118.80 |
| 24 | YA | 445 | C | N3-C2-O2 | -5.01 | 118.39 | 121.90 |
| 24 | YA | 974(A) | C | C2-N1-C1' | 5.01 | 124.31 | 118.80 |
| 24 | YA | 634 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 24 | YA | 1504 | C | N1-C2-O2 | 5.01 | 121.91 | 118.90 |
| 24 | YA | 2460 | U | N3-C2-O2 | -5.01 | 118.69 | 122.20 |
| 24 | YA | 1267 | U | N1-C2-O2 | 5.01 | 126.31 | 122.80 |
| 1 | QA | 410 | G | OP1-P-O3' | 5.01 | 116.22 | 105.20 |
| 24 | RA | 2874 | C | C2-N1-C1' | 5.01 | 124.31 | 118.80 |
| 24 | YA | 2720 | U | N1-C2-O2 | 5.01 | 126.31 | 122.80 |
| 24 | RA | 1294 | U | N1-C2-O2 | 5.01 | 126.31 | 122.80 |
| 10 | QJ | 90 | LEU | CA-CB-CG | 5.01 | 126.82 | 115.30 |
| 24 | RA | 2787 | C | N1-C2-O2 | 5.01 | 121.90 | 118.90 |
| 1 | XA | 58 | C | N1-C2-O2 | 5.01 | 121.90 | 118.90 |
| 24 | YA | 2594 | C | C6-N1-C2 | -5.00 | 118.30 | 120.30 |
| 24 | RA | 797 | C | C5-C6-N1 | 5.00 | 123.50 | 121.00 |
| 24 | RA | 1578 | U | N3-C2-O2 | -5.00 | 118.70 | 122.20 |
| 1 | XA | 754 | C | N1-C2-O2 | 5.00 | 121.90 | 118.90 |
| 24 | RA | 1022 | G | P-O3'-C3' | 5.00 | 125.70 | 119.70 |
| 24 | RA | 1830 | C | N1-C2-O2 | 5.00 | 121.90 | 118.90 |
| 1 | XA | 754 | C | C6-N1-C1' | -5.00 | 114.80 | 120.80 |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 4 | QD | 33 | MET | Peptide |
| 29 | RG | 82 | LEU | Peptide |
| 44 | RZ | 52 | SER | Peptide |
| 12 | XL | 104 | VAL | Peptide |
| 27 | YE | 17 | ASP | Peptide |
| 29 | YG | 82 | LEU | Peptide |
| 44 | YZ | 52 | SER | Peptide |

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | QA | 32247 | 0 | 16276 | 508 | 0 |
| 1 | XA | 32249 | 0 | 16279 | 516 | 1 |
| 2 | QB | 1907 | 0 | 1958 | 28 | 0 |
| 2 | XB | 1915 | 0 | 1969 | 33 | 0 |
| 3 | QC | 1605 | 0 | 1668 | 40 | 0 |
| 3 | XC | 1605 | 0 | 1668 | 27 | 1 |
| 4 | QD | 1703 | 0 | 1763 | 39 | 0 |
| 4 | XD | 1703 | 0 | 1763 | 53 | 1 |
| 5 | QE | 1155 | 0 | 1213 | 21 | 0 |
| 5 | XE | 1155 | 0 | 1213 | 24 | 0 |
| 6 | QF | 843 | 0 | 857 | 17 | 0 |
| 6 | XF | 843 | 0 | 857 | 9 | 0 |
| 7 | QG | 1257 | 0 | 1296 | 27 | 0 |
| 7 | XG | 1257 | 0 | 1296 | 22 | 0 |
| 8 | QH | 1108 | 0 | 1165 | 29 | 0 |
| 8 | XH | 1108 | 0 | 1165 | 30 | 0 |
| 9 | QI | 989 | 0 | 1011 | 29 | 0 |
| 9 | XI | 998 | 0 | 1024 | 26 | 0 |
| 10 | QJ | 801 | 0 | 849 | 26 | 0 |
| 10 | XJ | 777 | 0 | 816 | 27 | 0 |
| 11 | QK | 885 | 0 | 904 | 24 | 1 |
| 11 | XK | 864 | 0 | 881 | 17 | 0 |
| 12 | QL | 975 | 0 | 1062 | 29 | 0 |
| 12 | XL | 956 | 0 | 1046 | 18 | 0 |
| 13 | QM | 955 | 0 | 1021 | 38 | 0 |
| 13 | XM | 946 | 0 | 1008 | 20 | 0 |
| 14 | QN | 492 | 0 | 528 | 16 | 0 |
| 14 | XN | 492 | 0 | 531 | 36 | 0 |
| 15 | QO | 734 | 0 | 771 | 14 | 0 |
| 15 | XO | 729 | 0 | 768 | 11 | 0 |
| 16 | QP | 705 | 0 | 725 | 10 | 0 |
| 16 | XP | 705 | 0 | 725 | 9 | 0 |
| 17 | QQ | 834 | 0 | 904 | 11 | 0 |
| 17 | XQ | 834 | 0 | 904 | 18 | 0 |
| 18 | QR | 574 | 0 | 644 | 14 | 0 |
| 18 | XR | 574 | 0 | 644 | 12 | 0 |
| 19 | QS | 665 | 0 | 686 | 18 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19 | XS | 674 | 0 | 699 | 14 | 0 |
| 20 | QT | 763 | 0 | 861 | 15 | 0 |
| 20 | XT | 763 | 0 | 861 | 21 | 0 |
| 21 | QU | 217 | 0 | 234 | 5 | 0 |
| 21 | XU | 217 | 0 | 234 | 8 | 0 |
| 22 | QV | 1647 | 0 | 832 | 20 | 0 |
| 22 | XV | 1647 | 0 | 832 | 18 | 0 |
| 23 | QX | 418 | 0 | 209 | 10 | 0 |
| 23 | XX | 418 | 0 | 209 | 9 | 0 |
| 24 | RA | 62071 | 0 | 31291 | 830 | 4 |
| 24 | YA | 62091 | 0 | 31297 | 821 | 0 |
| 25 | RB | 2573 | 0 | 1306 | 27 | 0 |
| 25 | YB | 2573 | 0 | 1306 | 26 | 0 |
| 26 | RD | 2115 | 0 | 2195 | 50 | 0 |
| 26 | YD | 2115 | 0 | 2195 | 52 | 0 |
| 27 | RE | 1568 | 0 | 1634 | 53 | 0 |
| 27 | YE | 1568 | 0 | 1634 | 41 | 0 |
| 28 | RF | 1585 | 0 | 1632 | 25 | 0 |
| 28 | YF | 1585 | 0 | 1632 | 21 | 0 |
| 29 | RG | 1474 | 0 | 1535 | 33 | 0 |
| 29 | YG | 1474 | 0 | 1535 | 42 | 0 |
| 30 | RH | 1336 | 0 | 1418 | 33 | 0 |
| 30 | YH | 1336 | 0 | 1418 | 20 | 1 |
| 31 | RI | 1136 | 0 | 1223 | 15 | 0 |
| 31 | YI | 1136 | 0 | 1223 | 10 | 0 |
| 32 | RN | 1104 | 0 | 1180 | 23 | 0 |
| 32 | YN | 1104 | 0 | 1180 | 21 | 0 |
| 33 | RO | 933 | 0 | 996 | 23 | 0 |
| 33 | YO | 933 | 0 | 996 | 17 | 0 |
| 34 | RP | 1145 | 0 | 1228 | 35 | 0 |
| 34 | YP | 1122 | 0 | 1206 | 29 | 0 |
| 35 | RQ | 1122 | 0 | 1179 | 27 | 0 |
| 35 | YQ | 1122 | 0 | 1179 | 29 | 0 |
| 36 | RR | 960 | 0 | 1021 | 20 | 0 |
| 36 | YR | 960 | 0 | 1021 | 11 | 0 |
| 37 | RS | 882 | 0 | 942 | 19 | 0 |
| 37 | YS | 882 | 0 | 943 | 19 | 0 |
| 38 | RT | 1141 | 0 | 1202 | 26 | 0 |
| 38 | YT | 1141 | 0 | 1202 | 24 | 0 |
| 39 | RU | 964 | 0 | 1022 | 19 | 0 |
| 39 | YU | 964 | 0 | 1022 | 22 | 0 |
| 40 | RV | 779 | 0 | 852 | 18 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 40 | YV | 779 | 0 | 852 | 16 | 1 |
| 41 | RW | 900 | 0 | 964 | 16 | 0 |
| 41 | YW | 900 | 0 | 964 | 10 | 0 |
| 42 | RX | 725 | 0 | 778 | 9 | 0 |
| 42 | YX | 725 | 0 | 778 | 10 | 0 |
| 43 | RY | 818 | 0 | 909 | 16 | 0 |
| 43 | YY | 818 | 0 | 909 | 18 | 1 |
| 44 | RZ | 1461 | 0 | 1493 | 32 | 0 |
| 44 | YZ | 1461 | 0 | 1493 | 24 | 0 |
| 45 | R0 | 643 | 0 | 667 | 12 | 0 |
| 45 | Y0 | 593 | 0 | 612 | 15 | 0 |
| 46 | R1 | 763 | 0 | 848 | 11 | 0 |
| 46 | Y1 | 729 | 0 | 802 | 11 | 0 |
| 47 | R2 | 581 | 0 | 629 | 11 | 0 |
| 47 | Y2 | 581 | 0 | 629 | 9 | 2 |
| 48 | R3 | 469 | 0 | 518 | 6 | 0 |
| 48 | Y3 | 469 | 0 | 518 | 9 | 0 |
| 49 | R4 | 565 | 0 | 557 | 12 | 0 |
| 49 | Y4 | 565 | 0 | 557 | 21 | 0 |
| 50 | R5 | 459 | 0 | 476 | 16 | 0 |
| 50 | Y5 | 459 | 0 | 477 | 13 | 1 |
| 51 | R6 | 453 | 0 | 473 | 9 | 0 |
| 51 | Y6 | 453 | 0 | 473 | 11 | 0 |
| 52 | R7 | 409 | 0 | 454 | 4 | 0 |
| 52 | Y7 | 418 | 0 | 467 | 7 | 0 |
| 53 | R8 | 517 | 0 | 582 | 17 | 0 |
| 53 | Y8 | 517 | 0 | 582 | 19 | 0 |
| 54 | R9 | 307 | 0 | 335 | 9 | 0 |
| 54 | Y9 | 307 | 0 | 335 | 5 | 0 |
| 55 | QA | 69 | 0 | 0 | 0 | 0 |
| 55 | QE | 1 | 0 | 0 | 0 | 0 |
| 55 | QH | 1 | 0 | 0 | 0 | 0 |
| 55 | QV | 1 | 0 | 0 | 0 | 0 |
| 55 | R1 | 1 | 0 | 0 | 0 | 0 |
| 55 | RA | 381 | 0 | 0 | 0 | 0 |
| 55 | RB | 9 | 0 | 0 | 0 | 0 |
| 55 | RD | 1 | 0 | 0 | 0 | 0 |
| 55 | RE | 1 | 0 | 0 | 0 | 0 |
| 55 | RQ | 1 | 0 | 0 | 0 | 0 |
| 55 | XA | 67 | 0 | 0 | 0 | 0 |
| 55 | XE | 1 | 0 | 0 | 0 | 0 |
| 55 | Y0 | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 55 | Y5 | 1 | 0 | 0 | 0 | 0 |
| 55 | Y7 | 2 | 0 | 0 | 0 | 0 |
| 55 | YA | 454 | 0 | 0 | 0 | 0 |
| 55 | YB | 8 | 0 | 0 | 0 | 0 |
| 55 | YD | 2 | 0 | 0 | 0 | 0 |
| 55 | YE | 1 | 0 | 0 | 0 | 0 |
| 55 | YP | 1 | 0 | 0 | 0 | 0 |
| 55 | YQ | 2 | 0 | 0 | 0 | 0 |
| 55 | YR | 2 | 0 | 0 | 0 | 0 |
| 56 | QD | 8 | 0 | 0 | 1 | 0 |
| 56 | XD | 8 | 0 | 0 | 3 | 0 |
| 57 | QN | 1 | 0 | 0 | 0 | 0 |
| 57 | R4 | 1 | 0 | 0 | 0 | 0 |
| 57 | R5 | 1 | 0 | 0 | 0 | 0 |
| 57 | R6 | 1 | 0 | 0 | 0 | 0 |
| 57 | R9 | 1 | 0 | 0 | 0 | 0 |
| 57 | RY | 1 | 0 | 0 | 0 | 0 |
| 57 | XN | 1 | 0 | 0 | 0 | 0 |
| 57 | Y4 | 1 | 0 | 0 | 0 | 0 |
| 57 | Y5 | 1 | 0 | 0 | 0 | 0 |
| 57 | Y6 | 1 | 0 | 0 | 0 | 0 |
| 57 | Y9 | 1 | 0 | 0 | 0 | 0 |
| 57 | YY | 1 | 0 | 0 | 0 | 0 |
| All | All | 291782 | 0 | 197805 | 4186 | 7 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (4186) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:YN:24:CYS:SG | 14:YN:40:CYS:HB2 | 1.54 | 1.47 |
| 4:XD:61:LYS:CE | 4:XD:61:LYS:NZ | 1.77 | 1.47 |
| 14:YN:29:ARG:HD2 | 14:YN:40:CYS:SG | 1.67 | 1.33 |
| 14:YN:24:CYS:SG | 14:YN:40:CYS:CB | 2.36 | 1.14 |
| 14:YN:29:ARG:CD | 14:YN:40:CYS:SG | 2.36 | 1.13 |
| 24:RA:1657:C:O3' | 27:RE:133:LYS:HG2 | 1.62 | 0.99 |
| 24:RA:1473:G:H5'' | 24:RA:1473:G:H8 | 1.29 | 0.97 |
| 24:RA:2135:A:H62 | 24:RA:2156:G:H21 | 1.03 | 0.96 |
| 24:YA:1359:A:N6 | 24:YA:1372:U:H3 | 1.63 | 0.96 |
| 1:XA:152:A:N6 | 1:XA:169:C:N3 | 2.14 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:YY:76:CYS:HB3 | 43:YY:79:CYS:SG | 2.09 | 0.92 |
| 24:YA:1270:C:H5'' | 24:YA:1271:G:H5' | 1.52 | 0.90 |
| 24:YA:2701:C:H3' | 24:YA:2702:U:H5'' | 1.54 | 0.88 |
| 24:YA:2096:U:H3 | 24:YA:2193:G:H1 | 0.87 | 0.87 |
| 1:XA:452:A:H62 | 1:XA:480:U:H3 | 1.17 | 0.86 |
| 24:RA:1473:G:C8 | 24:RA:1473:G:H5'' | 2.11 | 0.86 |
| 10:XJ:50:ILE:H | 14:YN:41:ARG:HH12 | 1.22 | 0.86 |
| 24:RA:2675:A:H5' | 33:RO:31:LYS:HE3 | 1.57 | 0.85 |
| 24:YA:2099:U:H3 | 24:YA:2190:G:H1 | 1.17 | 0.85 |
| 24:YA:1359:A:H62 | 24:YA:1372:U:H3 | 0.89 | 0.85 |
| 24:RA:1264:G:OP1 | 50:R5:19:ARG:NH2 | 2.10 | 0.84 |
| 24:RA:1654:A:OP1 | 36:RR:2:ARG:HG2 | 1.78 | 0.84 |
| 51:R6:13:CYS:HB3 | 51:R6:16:CYS:SG | 2.18 | 0.83 |
| 14:YN:57:ARG:HE | 14:YN:58:LYS:H | 1.25 | 0.82 |
| 24:RA:1270:C:H5'' | 24:RA:1271:G:H5' | 1.59 | 0.82 |
| 16:QP:45:THR:HG22 | 16:QP:47:ASP:H | 1.43 | 0.82 |
| 1:XA:439:A:OP2 | 1:XA:493:G:N1 | 2.14 | 0.81 |
| 44:YZ:10:ARG:NH2 | 44:YZ:37:VAL:O | 2.14 | 0.81 |
| 24:RA:2135:A:H62 | 24:RA:2156:G:N2 | 1.78 | 0.81 |
| 24:RA:1657:C:O2' | 27:RE:133:LYS:HD2 | 1.80 | 0.80 |
| 24:RA:2135:A:N6 | 24:RA:2156:G:H21 | 1.78 | 0.80 |
| 44:YZ:5:LEU:H | 44:YZ:59:LEU:HA | 1.47 | 0.80 |
| 24:YA:2046:G:H5' | 50:Y5:19:ARG:HG3 | 1.64 | 0.79 |
| 24:YA:2245:U:H5' | 24:YA:2246:G:H5' | 1.64 | 0.79 |
| 24:RA:307:G:H2' | 24:RA:309:G:OP2 | 1.83 | 0.79 |
| 7:XG:62:PHE:HA | 7:XG:124:LEU:HD11 | 1.65 | 0.78 |
| 1:QA:939:G:H5' | 7:QG:102:ARG:HH12 | 1.49 | 0.78 |
| 44:YZ:52:SER:O | 44:YZ:54:HIS:N | 2.16 | 0.78 |
| 14:YN:24:CYS:SG | 14:YN:40:CYS:CA | 2.72 | 0.78 |
| 24:RA:527:C:N4 | 24:RA:2779:U:OP2 | 2.15 | 0.78 |
| 26:RD:8:PRO:HB3 | 26:RD:14:ARG:HB3 | 1.66 | 0.78 |
| 1:XA:1441:G:H21 | 1:XA:1460:A:H62 | 1.30 | 0.77 |
| 24:YA:2371:G:O2' | 51:Y6:46:HIS:ND1 | 2.17 | 0.77 |
| 7:XG:111:ARG:HH12 | 7:XG:123:GLU:N | 1.82 | 0.77 |
| 1:XA:686:U:H1' | 11:XK:42:TRP:HE1 | 1.49 | 0.77 |
| 14:YN:29:ARG:HD3 | 14:YN:40:CYS:SG | 2.25 | 0.77 |
| 24:YA:1800:C:OP2 | 26:YD:183:ARG:NH1 | 2.16 | 0.77 |
| 24:YA:1859:A:N6 | 24:YA:1883:G:O2' | 2.17 | 0.77 |
| 24:RA:1224:G:N2 | 24:RA:1227:A:OP2 | 2.17 | 0.76 |
| 24:RA:2245:U:H5' | 24:RA:2246:G:H5' | 1.67 | 0.76 |
| 44:RZ:5:LEU:HD21 | 44:RZ:47:VAL:HG21 | 1.68 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:RA:307:G:H8 | 24:RA:307:G:O5' | 1.68 | 0.76 |
| 1:XA:992:U:H3 | 1:XA:1044:A:H62 | 1.34 | 0.76 |
| 24:YA:2125:G:O2' | 24:YA:2173:A:N6 | 2.19 | 0.75 |
| 1:XA:157:G:H1 | 1:XA:164:U:H3 | 1.34 | 0.75 |
| 29:YG:67:LYS:HG3 | 49:Y4:5:ILE:HG12 | 1.68 | 0.75 |
| 24:YA:1055:G:H1 | 24:YA:1104:C:H42 | 1.34 | 0.74 |
| 1:QA:559:A:H4' | 1:QA:560:U:H5'' | 1.68 | 0.74 |
| 1:QA:674:G:H2' | 1:QA:675:A:H8 | 1.53 | 0.74 |
| 22:XV:19:G:O2' | 22:XV:58:G:N2 | 2.20 | 0.74 |
| 24:RA:1817:G:OP1 | 26:RD:88:ARG:NH2 | 2.21 | 0.74 |
| 13:XM:99:ARG:HB3 | 13:XM:101:GLN:HE22 | 1.51 | 0.74 |
| 1:XA:1236:A:H4' | 1:XA:1304:G:H4' | 1.68 | 0.74 |
| 26:YD:8:PRO:HB3 | 26:YD:14:ARG:HB3 | 1.70 | 0.74 |
| 24:YA:2134:A:N6 | 24:YA:2156:G:O2' | 2.21 | 0.73 |
| 24:YA:2584:U:H2' | 24:YA:2585:U:H2' | 1.70 | 0.73 |
| 24:RA:2406:U:OP1 | 24:RA:2411:A:N6 | 2.21 | 0.73 |
| 24:RA:527:C:N3 | 24:RA:2779:U:H5'' | 2.03 | 0.73 |
| 1:QA:618:C:H5' | 1:QA:619:U:H5'' | 1.70 | 0.73 |
| 8:QH:29:SER:HB3 | 8:QH:32:LYS:HE2 | 1.69 | 0.73 |
| 5:XE:102:ALA:HB1 | 5:XE:106:PRO:HG2 | 1.68 | 0.73 |
| 48:Y3:38:GLU:OE2 | 48:Y3:38:GLU:N | 2.14 | 0.73 |
| 24:YA:1607:C:N4 | 24:YA:1622:G:OP2 | 2.21 | 0.73 |
| 24:YA:2581:G:OP2 | 24:YA:2581:G:N2 | 2.19 | 0.73 |
| 24:RA:1638:C:H5'' | 24:RA:2710:C:O2' | 1.89 | 0.72 |
| 12:XL:60:LEU:HD12 | 12:XL:62:SER:H | 1.54 | 0.72 |
| 24:YA:994:C:OP1 | 39:YU:53:ARG:NH2 | 2.23 | 0.72 |
| 1:XA:978:A:OP2 | 1:XA:1362(A):C:N4 | 2.20 | 0.72 |
| 9:XI:20:ARG:HE | 9:XI:21:PRO:HD2 | 1.54 | 0.71 |
| 24:YA:783:A:H2' | 24:YA:784:A:H4' | 1.72 | 0.71 |
| 1:XA:410:G:H21 | 1:XA:432:A:H62 | 1.37 | 0.71 |
| 24:YA:888:C:H3' | 24:YA:889:C:H4' | 1.72 | 0.71 |
| 14:QN:27:CYS:SG | 14:QN:40:CYS:HB3 | 2.30 | 0.71 |
| 1:XA:1123:A:H4' | 10:XJ:36:GLY:HA3 | 1.71 | 0.71 |
| 1:XA:1422:G:H5'' | 33:YO:48:PRO:HB3 | 1.73 | 0.71 |
| 44:RZ:5:LEU:H | 44:RZ:59:LEU:HA | 1.54 | 0.71 |
| 1:XA:674:G:H2' | 1:XA:675:A:H8 | 1.55 | 0.71 |
| 24:YA:1817:G:OP1 | 26:YD:88:ARG:NH2 | 2.24 | 0.71 |
| 25:RB:80:U:H2' | 25:RB:81:G:H21 | 1.54 | 0.71 |
| 14:XN:29:ARG:HD2 | 14:XN:40:CYS:HG | 1.54 | 0.71 |
| 14:XN:27:CYS:SG | 14:XN:40:CYS:CB | 2.78 | 0.71 |
| 24:RA:2046:G:H5' | 50:R5:19:ARG:HG3 | 1.73 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:YN:27:CYS:SG | 14:YN:40:CYS:HB2 | 2.31 | 0.71 |
| 24:YA:517:C:OP1 | 50:Y5:16:ARG:NH2 | 2.24 | 0.71 |
| 11:QK:93:GLN:OE1 | 11:QK:96:ARG:NH2 | 2.24 | 0.71 |
| 24:RA:392:C:H5'' | 24:RA:409:C:H5'' | 1.71 | 0.71 |
| 1:QA:1077:G:N2 | 1:QA:1080:A:OP2 | 2.21 | 0.70 |
| 1:QA:339:C:OP2 | 33:RO:97:ARG:NH1 | 2.20 | 0.70 |
| 1:QA:1123:A:H4' | 10:QJ:36:GLY:HA3 | 1.72 | 0.70 |
| 24:RA:2688:U:OP1 | 24:RA:2713:A:N6 | 2.23 | 0.70 |
| 24:RA:994:C:OP1 | 39:RU:53:ARG:NH2 | 2.24 | 0.70 |
| 44:RZ:52:SER:O | 44:RZ:54:HIS:N | 2.20 | 0.70 |
| 25:RB:33:G:H5' | 29:RG:2:PRO:HG3 | 1.73 | 0.70 |
| 1:XA:261:U:OP2 | 20:XT:79:ARG:NH2 | 2.25 | 0.70 |
| 1:XA:689:C:H3' | 1:XA:690:G:H21 | 1.56 | 0.70 |
| 46:R1:76:ARG:HH11 | 46:R1:94:LEU:HD23 | 1.57 | 0.70 |
| 24:YA:1026:U:H4' | 24:YA:1027:A:OP1 | 1.92 | 0.70 |
| 1:XA:403:C:OP2 | 4:XD:74:GLN:NE2 | 2.24 | 0.70 |
| 24:YA:1670:C:C5' | 24:YA:1671:U:OP2 | 2.40 | 0.70 |
| 1:XA:1318:A:H4' | 19:XS:11:VAL:HG21 | 1.74 | 0.69 |
| 24:YA:288:C:H2' | 24:YA:289:A:H8 | 1.57 | 0.69 |
| 24:YA:620:G:H4' | 24:YA:621:A:H5'' | 1.73 | 0.69 |
| 24:YA:67:U:H3 | 24:YA:74:A:H2 | 1.39 | 0.69 |
| 24:RA:140:A:H8 | 24:RA:1408:C:HO2' | 1.41 | 0.69 |
| 24:RA:630:G:N2 | 24:RA:633:A:OP2 | 2.25 | 0.69 |
| 25:RB:30:C:H1' | 25:RB:57:A:H61 | 1.56 | 0.69 |
| 1:QA:838:G:H1 | 1:QA:848:C:H42 | 1.38 | 0.69 |
| 24:RA:994:C:OP2 | 39:RU:54:LYS:NZ | 2.25 | 0.69 |
| 38:YT:125:ARG:HE | 38:YT:129:ARG:HH12 | 1.39 | 0.69 |
| 5:QE:102:ALA:HB1 | 5:QE:106:PRO:HG2 | 1.74 | 0.69 |
| 14:QN:27:CYS:SG | 14:QN:40:CYS:CB | 2.80 | 0.69 |
| 24:YA:512:G:OP1 | 24:YA:1234:U:O2' | 2.10 | 0.69 |
| 1:QA:782:A:H62 | 1:QA:800:G:H21 | 1.40 | 0.69 |
| 24:RA:2115:G:N1 | 24:RA:2164:C:OP2 | 2.26 | 0.69 |
| 1:XA:618:C:H5' | 1:XA:619:U:H5'' | 1.73 | 0.69 |
| 24:YA:1670:C:H5'' | 24:YA:1671:U:OP2 | 1.93 | 0.69 |
| 24:YA:571:A:H5' | 24:YA:2030:A:H62 | 1.57 | 0.69 |
| 1:XA:1227:A:OP1 | 19:XS:80:TYR:OH | 2.10 | 0.69 |
| 24:YA:1012:U:O2' | 24:YA:1013:C:OP2 | 2.11 | 0.69 |
| 24:YA:1509:C:H3' | 24:YA:1510:A:H5'' | 1.74 | 0.69 |
| 1:XA:1348:U:H4' | 9:XI:120:ARG:HD2 | 1.74 | 0.69 |
| 9:XI:9:ARG:HG3 | 9:XI:104:ARG:HH21 | 1.56 | 0.69 |
| 1:XA:677:U:H3 | 1:XA:713:G:H22 | 1.41 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:QA:1400:C:O4' | 23:QX:21:G:C6 | 2.46 | 0.69 |
| 1:QA:689:C:H3' | 1:QA:690:G:H21 | 1.57 | 0.69 |
| 1:QA:1306:A:N6 | 1:QA:1331:G:O2' | 2.25 | 0.69 |
| 1:XA:1157:A:N7 | 1:XA:1178:G:N2 | 2.40 | 0.69 |
| 3:XC:6:HIS:CE1 | 3:XC:8:ILE:HB | 2.28 | 0.69 |
| 24:YA:996:A:OP2 | 39:YU:92:ARG:NH2 | 2.27 | 0.68 |
| 1:QA:1504:G:OP1 | 1:QA:1507:A:O2' | 2.10 | 0.68 |
| 24:RA:993:G:OP1 | 39:RU:50:ARG:NH2 | 2.25 | 0.68 |
| 54:Y9:13:LYS:HD2 | 54:Y9:28:GLU:H | 1.57 | 0.68 |
| 24:YA:1012:U:C2' | 24:YA:1013:C:OP2 | 2.41 | 0.68 |
| 24:YA:2154:G:H2' | 24:YA:2155:G:H8 | 1.57 | 0.68 |
| 24:YA:1030:G:OP2 | 35:YQ:128:LYS:NZ | 2.26 | 0.68 |
| 24:RA:1433:U:H3 | 24:RA:1560:G:H1 | 1.41 | 0.68 |
| 28:RF:158:THR:O | 28:RF:164:ARG:NH1 | 2.26 | 0.68 |
| 24:RA:309:G:OP2 | 24:RA:309:G:C8 | 2.46 | 0.68 |
| 24:RA:141:A:H8 | 24:RA:1595:G:H21 | 1.42 | 0.68 |
| 29:RG:29:TRP:O | 29:RG:33:ARG:NH1 | 2.27 | 0.68 |
| 24:YA:1359:A:N7 | 24:YA:1372:U:O4 | 2.26 | 0.68 |
| 24:YA:1728:G:N1 | 24:YA:1730:U:OP2 | 2.26 | 0.68 |
| 1:QA:261:U:OP2 | 20:QT:79:ARG:NH2 | 2.27 | 0.68 |
| 1:XA:264:U:O2' | 17:XQ:64:PRO:O | 2.11 | 0.68 |
| 38:YT:5:ALA:HA | 38:YT:8:LYS:HD3 | 1.74 | 0.68 |
| 1:QA:811:C:O2' | 1:QA:901:A:N1 | 2.27 | 0.68 |
| 4:XD:61:LYS:CD | 4:XD:61:LYS:NZ | 2.55 | 0.68 |
| 1:QA:1305:G:HO2' | 1:QA:1306:A:H8 | 1.41 | 0.67 |
| 10:QJ:3:LYS:N | 10:QJ:74:ILE:O | 2.27 | 0.67 |
| 1:XA:1266:G:N2 | 1:XA:1269:A:OP2 | 2.21 | 0.67 |
| 24:YA:1110:G:H4' | 30:YH:3:ARG:HE | 1.60 | 0.67 |
| 24:YA:2291:U:H3 | 24:YA:2341:G:H1 | 1.42 | 0.67 |
| 24:YA:2788:C:O2' | 24:YA:2809:A:N3 | 2.26 | 0.67 |
| 3:XC:18:TRP:O | 3:XC:21:ARG:NH2 | 2.27 | 0.67 |
| 24:RA:2711:A:H5'' | 24:RA:2712:U:H5'' | 1.75 | 0.67 |
| 35:RQ:65:PHE:HB2 | 35:RQ:105:GLU:HB3 | 1.75 | 0.67 |
| 24:YA:2296:U:OP2 | 37:YS:9:ARG:NH1 | 2.28 | 0.67 |
| 24:YA:2821:A:OP2 | 24:YA:2822:G:OP2 | 2.11 | 0.67 |
| 1:QA:45:U:H3 | 1:QA:396:G:H1 | 1.43 | 0.67 |
| 3:XC:85:ARG:HA | 3:XC:88:ARG:HE | 1.59 | 0.67 |
| 24:RA:2285:C:OP2 | 51:R6:6:ARG:NH1 | 2.28 | 0.67 |
| 1:XA:553:A:H5'' | 12:XL:24:VAL:HG21 | 1.76 | 0.67 |
| 1:XA:812:C:H4' | 1:XA:813:U:H5' | 1.75 | 0.67 |
| 5:XE:75:THR:OG1 | 5:XE:76:ILE:N | 2.28 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:YA:593:G:H4' | 53:Y8:61:LEU:HD13 | 1.77 | 0.67 |
| 24:YA:1728:G:H8 | 24:YA:1732:A:H62 | 1.43 | 0.66 |
| 34:YP:65:ARG:HE | 53:Y8:15:LYS:HB2 | 1.60 | 0.66 |
| 12:XL:114:LYS:O | 12:XL:117:ARG:NH1 | 2.28 | 0.66 |
| 46:Y1:83:GLU:HG2 | 46:Y1:85:LEU:H | 1.60 | 0.66 |
| 44:YZ:4:ARG:HB3 | 44:YZ:60:GLU:HG3 | 1.78 | 0.66 |
| 1:QA:806:C:H2' | 1:QA:807:A:H8 | 1.61 | 0.66 |
| 5:QE:75:THR:OG1 | 5:QE:76:ILE:N | 2.28 | 0.66 |
| 24:RA:676:A:H8 | 24:RA:2069:G:H21 | 1.43 | 0.66 |
| 24:RA:27:G:N2 | 24:RA:513:A:OP2 | 2.29 | 0.66 |
| 1:QA:1222:G:OP1 | 19:QS:78:ARG:NH1 | 2.27 | 0.66 |
| 49:Y4:46:GLN:HG3 | 49:Y4:48:ARG:HE | 1.60 | 0.66 |
| 24:RA:309:G:N3 | 24:RA:329:G:O2' | 2.28 | 0.66 |
| 1:XA:261:U:N3 | 1:XA:264:U:OP2 | 2.28 | 0.66 |
| 19:XS:19:VAL:HG21 | 19:XS:44:MET:HG2 | 1.78 | 0.66 |
| 24:YA:850:C:N4 | 24:YA:929:G:N2 | 2.43 | 0.66 |
| 51:R6:13:CYS:CB | 51:R6:16:CYS:SG | 2.82 | 0.66 |
| 1:QA:316:G:OP2 | 1:QA:351:G:O2' | 2.13 | 0.66 |
| 5:QE:35:GLY:HA3 | 5:QE:112:LEU:HB3 | 1.76 | 0.66 |
| 14:QN:24:CYS:CB | 14:QN:27:CYS:SG | 2.79 | 0.66 |
| 24:RA:2747:G:H21 | 24:RA:2757:A:H62 | 1.42 | 0.66 |
| 33:RO:104:ARG:HH11 | 33:RO:121:VAL:HG22 | 1.61 | 0.66 |
| 51:Y6:13:CYS:HB3 | 51:Y6:16:CYS:SG | 2.35 | 0.66 |
| 1:QA:1347:G:N2 | 1:QA:1374:A:OP2 | 2.24 | 0.66 |
| 22:QV:19:G:O2' | 22:QV:58:G:N2 | 2.29 | 0.66 |
| 24:RA:2638:G:OP1 | 27:RE:82:ARG:NH2 | 2.29 | 0.66 |
| 34:YP:58:THR:O | 34:YP:61:ARG:NH2 | 2.28 | 0.66 |
| 1:QA:553:A:H5'' | 12:QL:24:VAL:HG11 | 1.78 | 0.66 |
| 1:QA:677:U:H3 | 1:QA:713:G:H22 | 1.40 | 0.66 |
| 1:XA:946:A:O2' | 1:XA:1333:A:N3 | 2.29 | 0.66 |
| 24:YA:141:A:H8 | 24:YA:1595:G:H21 | 1.42 | 0.65 |
| 1:QA:1023:G:H3' | 1:QA:1024:G:H5'' | 1.79 | 0.65 |
| 24:YA:630:G:OP1 | 53:Y8:46:ARG:NH1 | 2.30 | 0.65 |
| 1:QA:1522:U:H2' | 1:QA:1523:G:H8 | 1.62 | 0.65 |
| 1:XA:579:G:H5' | 1:XA:728:A:H1' | 1.76 | 0.65 |
| 1:XA:662:G:O2' | 1:XA:836:G:OP1 | 2.15 | 0.65 |
| 2:QB:54:THR:HG22 | 2:QB:199:TYR:HB3 | 1.77 | 0.65 |
| 14:XN:24:CYS:CB | 14:XN:27:CYS:SG | 2.85 | 0.65 |
| 51:Y6:10:LEU:HD23 | 51:Y6:19:ARG:HG2 | 1.78 | 0.65 |
| 1:QA:953:G:N7 | 13:QM:104:ARG:NH2 | 2.44 | 0.65 |
| 3:QC:173:VAL:HG22 | 3:QC:203:PHE:HB2 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:581:G:N1 | 1:XA:759:A:OP2 | 2.28 | 0.65 |
| 14:YN:24:CYS:SG | 14:YN:40:CYS:N | 2.70 | 0.65 |
| 37:YS:20:ARG:NH2 | 45:Y0:51:VAL:O | 2.26 | 0.65 |
| 1:QA:439:A:OP2 | 1:QA:493:G:N1 | 2.29 | 0.65 |
| 24:RA:1607:C:N4 | 24:RA:1622:G:OP2 | 2.29 | 0.65 |
| 2:XB:54:THR:HG22 | 2:XB:199:TYR:HB3 | 1.78 | 0.65 |
| 21:XU:12:LYS:HB3 | 21:XU:22:ARG:HD3 | 1.79 | 0.65 |
| 24:RA:26:G:H1' | 24:RA:515:A:H61 | 1.62 | 0.65 |
| 24:RA:2816:C:O2 | 24:RA:2883:A:O2' | 2.14 | 0.65 |
| 1:XA:324:G:O5' | 1:XA:324:G:H8 | 1.80 | 0.65 |
| 1:XA:745:C:H2' | 1:XA:746:A:H8 | 1.61 | 0.65 |
| 8:XH:111:ILE:HG23 | 8:XH:134:ILE:HB | 1.78 | 0.65 |
| 53:Y8:29:LYS:O | 53:Y8:31:HIS:N | 2.30 | 0.65 |
| 24:RA:987:G:O2' | 24:RA:1000:A:N3 | 2.30 | 0.65 |
| 24:YA:2010:G:H5'' | 41:YW:42:ARG:HB2 | 1.79 | 0.64 |
| 24:YA:527:C:N4 | 24:YA:2779:U:OP2 | 2.31 | 0.64 |
| 24:YA:2729:G:H1' | 27:YE:187:ALA:HB2 | 1.79 | 0.64 |
| 24:RA:1365:A:O2' | 46:R1:11:ARG:NH2 | 2.30 | 0.64 |
| 1:XA:235:C:H2' | 1:XA:236:G:H8 | 1.63 | 0.64 |
| 24:YA:807:U:O2' | 24:YA:2060:A:N1 | 2.29 | 0.64 |
| 4:XD:9:CYS:SG | 4:XD:25:ARG:NH1 | 2.68 | 0.64 |
| 1:QA:1301:U:O3' | 13:QM:21:TYR:OH | 2.14 | 0.64 |
| 5:QE:79:GLU:HB3 | 5:QE:92:LYS:HD3 | 1.79 | 0.64 |
| 24:RA:2296:U:OP2 | 37:RS:9:ARG:NH1 | 2.30 | 0.64 |
| 10:XJ:50:ILE:HA | 10:XJ:60:ARG:HG3 | 1.79 | 0.64 |
| 11:QK:18:ARG:HG2 | 11:QK:81:ASP:HB2 | 1.80 | 0.64 |
| 22:QV:4:U:HO2' | 22:QV:5:G:H8 | 1.43 | 0.64 |
| 24:RA:768:G:O2' | 24:RA:1379:A:N6 | 2.30 | 0.64 |
| 26:RD:124:PRO:HB2 | 26:RD:126:GLN:HE22 | 1.63 | 0.64 |
| 24:RA:2882:A:OP1 | 36:RR:96:ARG:NH1 | 2.31 | 0.64 |
| 43:RY:14:LEU:HB2 | 43:RY:75:ILE:HD11 | 1.80 | 0.64 |
| 1:XA:578:C:O2' | 1:XA:728:A:N3 | 2.29 | 0.64 |
| 29:YG:67:LYS:HE3 | 49:Y4:7:PRO:HD3 | 1.78 | 0.64 |
| 24:YA:993:G:OP1 | 39:YU:50:ARG:NH2 | 2.31 | 0.64 |
| 40:YV:61:VAL:HG12 | 40:YV:63:GLY:H | 1.63 | 0.64 |
| 2:XB:219:VAL:HA | 2:XB:222:ILE:HD12 | 1.80 | 0.64 |
| 1:QA:343:U:O2 | 1:QA:346:G:N2 | 2.28 | 0.64 |
| 9:QI:112:LYS:NZ | 9:QI:113:LYS:O | 2.30 | 0.64 |
| 30:YH:151:ILE:O | 30:YH:153:LYS:N | 2.30 | 0.64 |
| 1:QA:1116:C:H2' | 1:QA:1117:G:H8 | 1.63 | 0.64 |
| 3:XC:11:ARG:NH2 | 3:XC:177:THR:O | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:XD:100:ARG:NH2 | 4:XD:136:PRO:O | 2.31 | 0.64 |
| 24:YA:1316:U:H2' | 24:YA:1317:A:H8 | 1.62 | 0.64 |
| 25:YB:30:C:H1' | 25:YB:57:A:H61 | 1.63 | 0.64 |
| 1:QA:1373:G:H5' | 7:QG:36:LYS:HG2 | 1.80 | 0.64 |
| 13:QM:91:ARG:HH21 | 13:QM:96:LEU:HB3 | 1.63 | 0.64 |
| 24:RA:308:G:O2' | 24:RA:329:G:N2 | 2.31 | 0.64 |
| 24:RA:998:C:OP2 | 39:RU:58:ARG:NH1 | 2.30 | 0.64 |
| 1:XA:521:G:HO2' | 1:XA:536:C:HO2' | 1.45 | 0.64 |
| 2:XB:118:LEU:HD21 | 2:XB:142:LEU:HA | 1.80 | 0.64 |
| 14:XN:24:CYS:SG | 14:XN:33:VAL:HG22 | 2.38 | 0.64 |
| 24:YA:2328:A:H2' | 24:YA:2329:G:C8 | 2.33 | 0.64 |
| 24:YA:589:C:H2' | 24:YA:590:A:H8 | 1.62 | 0.64 |
| 1:QA:745:C:OP1 | 1:QA:851:G:O2' | 2.16 | 0.63 |
| 1:XA:707:C:OP1 | 11:XK:85:ARG:NH1 | 2.31 | 0.63 |
| 20:XT:58:LYS:O | 20:XT:61:SER:OG | 2.15 | 0.63 |
| 1:QA:514:C:H2' | 1:QA:515:G:H8 | 1.63 | 0.63 |
| 24:RA:67:U:H6 | 24:RA:67:U:O5' | 1.80 | 0.63 |
| 1:XA:380:G:N2 | 1:XA:383:A:OP2 | 2.25 | 0.63 |
| 1:XA:544:G:OP1 | 4:XD:59:ARG:NH2 | 2.30 | 0.63 |
| 51:Y6:13:CYS:CB | 51:Y6:16:CYS:SG | 2.79 | 0.63 |
| 1:XA:1253:G:H4' | 10:XJ:46:ARG:HH12 | 1.64 | 0.63 |
| 20:XT:14:LYS:HA | 20:XT:17:ARG:HD3 | 1.80 | 0.63 |
| 24:YA:2646:C:OP2 | 24:YA:2732:G:O2' | 2.10 | 0.63 |
| 10:QJ:19:SER:HA | 10:QJ:22:LYS:HD2 | 1.79 | 0.63 |
| 24:RA:776:G:N1 | 24:RA:2072:G:OP1 | 2.30 | 0.63 |
| 24:RA:587:C:OP2 | 34:RP:21:ARG:NH1 | 2.31 | 0.63 |
| 1:XA:953:G:N7 | 13:XM:104:ARG:NH2 | 2.46 | 0.63 |
| 24:YA:2068:U:H3 | 24:YA:2430:A:H2 | 1.43 | 0.63 |
| 24:YA:270(I):G:H1 | 24:YA:270(Q):C:H42 | 1.46 | 0.63 |
| 24:YA:694:U:H3 | 24:YA:768:G:H1 | 1.44 | 0.63 |
| 27:YE:17:ASP:O | 27:YE:19:ARG:N | 2.32 | 0.63 |
| 26:RD:13:ARG:NH1 | 26:RD:16:MET:SD | 2.71 | 0.63 |
| 34:RP:58:THR:O | 34:RP:61:ARG:NH2 | 2.31 | 0.63 |
| 24:YA:2680:C:H5' | 27:YE:189:PRO:HA | 1.80 | 0.63 |
| 24:RA:1509:C:H3' | 24:RA:1510:A:H5'' | 1.79 | 0.63 |
| 1:XA:358:U:H2' | 1:XA:359:U:C6 | 2.34 | 0.63 |
| 24:RA:1152:C:H2' | 24:RA:1153:C:H6 | 1.63 | 0.63 |
| 1:XA:1224:G:O2' | 1:XA:1322:C:OP2 | 2.17 | 0.63 |
| 9:XI:121:ARG:NH1 | 9:XI:122:ALA:O | 2.32 | 0.63 |
| 24:YA:277:C:C5' | 24:YA:278:A:H5' | 2.29 | 0.63 |
| 1:QA:1305:G:N2 | 1:QA:1332:A:OP2 | 2.32 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:QJ:41:PRO:HB2 | 10:QJ:43:ARG:HH22 | 1.63 | 0.62 |
| 13:QM:25:ILE:HD11 | 13:QM:66:LEU:HD11 | 1.79 | 0.62 |
| 24:YA:919:G:N2 | 24:YA:2269:A:OP2 | 2.32 | 0.62 |
| 24:RA:2228:G:OP1 | 26:RD:261:LYS:NZ | 2.25 | 0.62 |
| 24:RA:883:G:H1 | 24:RA:893:C:H42 | 1.47 | 0.62 |
| 27:RE:17:ASP:O | 27:RE:19:ARG:N | 2.30 | 0.62 |
| 13:XM:57:ARG:HH22 | 49:Y4:34:GLU:HB2 | 1.64 | 0.62 |
| 24:YA:1264:G:OP1 | 50:Y5:19:ARG:NH2 | 2.19 | 0.62 |
| 1:XA:714:G:H2' | 1:XA:715:A:C8 | 2.34 | 0.62 |
| 1:XA:715:A:H2' | 1:XA:716:A:C8 | 2.34 | 0.62 |
| 24:YA:2287:A:H62 | 24:YA:2344:U:H3 | 1.46 | 0.62 |
| 24:YA:270:A:OP2 | 24:YA:270(Y):G:N1 | 2.31 | 0.62 |
| 39:RU:92:ARG:HD2 | 40:RV:11:GLN:HB2 | 1.80 | 0.62 |
| 1:XA:1305:G:N2 | 1:XA:1332:A:OP2 | 2.32 | 0.62 |
| 1:QA:1224:G:O2' | 1:QA:1322:C:OP2 | 2.18 | 0.62 |
| 8:QH:32:LYS:HA | 8:QH:35:ILE:HD12 | 1.81 | 0.62 |
| 24:RA:1882:C:H3' | 24:RA:1883:G:H8 | 1.65 | 0.62 |
| 24:YA:1980:G:O2' | 24:YA:1982:C:OP2 | 2.15 | 0.62 |
| 10:QJ:40:LEU:HD11 | 10:QJ:71:LEU:HG | 1.80 | 0.62 |
| 24:RA:1083:U:H2' | 24:RA:1085:A:H5'' | 1.81 | 0.62 |
| 35:RQ:81:VAL:O | 35:RQ:82:ARG:NE | 2.28 | 0.62 |
| 1:XA:1141:C:H2' | 1:XA:1142:G:H8 | 1.64 | 0.62 |
| 27:RE:176:ILE:HB | 27:RE:181:LEU:HB2 | 1.81 | 0.62 |
| 28:RF:117:ARG:NH2 | 28:RF:189:THR:O | 2.33 | 0.62 |
| 4:XD:25:ARG:NH1 | 56:XD:301:SF4:S2 | 2.73 | 0.62 |
| 1:QA:581:G:OP1 | 15:QO:65:ARG:NH1 | 2.30 | 0.62 |
| 5:QE:43:LEU:HD21 | 5:QE:109:ILE:HD12 | 1.80 | 0.62 |
| 24:RA:270(T):G:H5'' | 46:R1:97:LEU:HD22 | 1.81 | 0.62 |
| 24:RA:1859:A:N6 | 24:RA:1883:G:O2' | 2.33 | 0.62 |
| 26:RD:143:HIS:ND1 | 26:RD:194:GLY:O | 2.27 | 0.62 |
| 1:XA:1073:U:O2' | 2:XB:104:ASN:OD1 | 2.17 | 0.62 |
| 24:YA:1127:A:N7 | 24:YA:2488:A:O2' | 2.31 | 0.62 |
| 24:YA:265:A:N6 | 24:YA:427:U:O2' | 2.32 | 0.62 |
| 1:QA:714:G:H2' | 1:QA:715:A:C8 | 2.34 | 0.62 |
| 24:RA:517:C:OP1 | 50:R5:16:ARG:NH2 | 2.32 | 0.62 |
| 24:RA:2118:U:O2 | 24:RA:2148:G:O2' | 2.17 | 0.62 |
| 1:XA:1522:U:H2' | 1:XA:1523:G:H8 | 1.65 | 0.62 |
| 1:QA:1343:G:H4' | 9:QI:122:ALA:HB3 | 1.81 | 0.62 |
| 24:RA:1652:A:OP1 | 36:RR:8:ARG:NH1 | 2.33 | 0.62 |
| 30:RH:153:LYS:HB2 | 30:RH:162:ILE:HG12 | 1.80 | 0.62 |
| 24:YA:577:G:O2' | 24:YA:1254:A:OP1 | 2.18 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:QA:579:G:H5' | 1:QA:728:A:H1' | 1.81 | 0.61 |
| 15:QO:25:THR:HB | 15:QO:70:LEU:HD21 | 1.82 | 0.61 |
| 47:R2:54:LYS:HA | 47:R2:57:ILE:HD12 | 1.82 | 0.61 |
| 1:XA:673:G:H2' | 1:XA:674:G:C8 | 2.35 | 0.61 |
| 9:XI:111:ARG:NH1 | 9:XI:112:LYS:O | 2.33 | 0.61 |
| 24:RA:2199:A:OP1 | 46:R1:50:ARG:NH2 | 2.32 | 0.61 |
| 1:XA:1251:A:N3 | 1:XA:1369:C:O2' | 2.32 | 0.61 |
| 2:XB:92:TYR:HE2 | 2:XB:94:ASN:HD22 | 1.47 | 0.61 |
| 3:QC:70:VAL:HG12 | 3:QC:72:LYS:H | 1.66 | 0.61 |
| 1:XA:191(G):G:O2' | 20:XT:101:GLY:O | 2.18 | 0.61 |
| 1:QA:543:C:OP2 | 4:QD:10:ARG:NH1 | 2.33 | 0.61 |
| 10:QJ:30:SER:O | 10:QJ:78:ASN:ND2 | 2.34 | 0.61 |
| 24:RA:1969:A:O2' | 24:RA:1972:A:N3 | 2.30 | 0.61 |
| 24:RA:530:G:N1 | 24:RA:2022:U:OP1 | 2.33 | 0.61 |
| 24:YA:1530:G:O6 | 24:YA:1542:G:N2 | 2.32 | 0.61 |
| 24:YA:372:G:N2 | 24:YA:401:A:OP2 | 2.33 | 0.61 |
| 25:YB:22:U:H3 | 25:YB:61:G:H1 | 1.48 | 0.61 |
| 25:YB:80:U:H2' | 25:YB:81:G:H21 | 1.64 | 0.61 |
| 34:YP:37:GLY:N | 34:YP:40:SER:OG | 2.33 | 0.61 |
| 44:YZ:53:ILE:HG22 | 44:YZ:71:VAL:HG13 | 1.83 | 0.61 |
| 1:QA:1119:C:H2' | 1:QA:1120:G:H8 | 1.66 | 0.61 |
| 24:RA:1521:G:H5'' | 24:RA:1521:G:H8 | 1.66 | 0.61 |
| 24:RA:2365:G:O6 | 53:R8:43:GLN:NE2 | 2.33 | 0.61 |
| 24:YA:1026:U:C4' | 24:YA:1027:A:OP1 | 2.48 | 0.61 |
| 24:YA:2224:G:OP1 | 26:YD:268:ARG:NH1 | 2.33 | 0.61 |
| 24:YA:392:C:H5'' | 24:YA:409:C:H5'' | 1.82 | 0.61 |
| 4:QD:25:ARG:NH1 | 56:QD:301:SF4:S3 | 2.74 | 0.61 |
| 27:RE:201:THR:HG22 | 27:RE:203:LYS:H | 1.65 | 0.61 |
| 1:XA:363:A:OP1 | 12:XL:34:ARG:N | 2.29 | 0.61 |
| 24:YA:1019:U:H3 | 24:YA:1142(A):A:H62 | 1.49 | 0.61 |
| 24:RA:546:C:H3' | 24:RA:547:A:H8 | 1.66 | 0.61 |
| 1:XA:1356:G:H2' | 1:XA:1357:A:C8 | 2.36 | 0.61 |
| 1:XA:1446:A:O2' | 1:XA:1447:G:O5' | 2.16 | 0.61 |
| 22:XV:59:A:O2' | 22:XV:61:U:OP2 | 2.13 | 0.61 |
| 49:R4:58:ARG:HA | 49:R4:61:ARG:HH21 | 1.66 | 0.61 |
| 24:RA:1058:G:N2 | 24:RA:1080:C:O2 | 2.34 | 0.61 |
| 24:RA:1138:G:O2' | 32:RN:102:ALA:O | 2.19 | 0.61 |
| 12:XL:89:ARG:NH2 | 12:XL:93:LEU:O | 2.33 | 0.61 |
| 17:XQ:66:SER:O | 17:XQ:70:ARG:NH1 | 2.34 | 0.61 |
| 1:XA:192:U:O2' | 20:XT:60:GLU:OE2 | 2.17 | 0.61 |
| 35:YQ:65:PHE:HB2 | 35:YQ:105:GLU:HB3 | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:RA:1636:C:H2' | 24:RA:1637:A:C8 | 2.36 | 0.61 |
| 24:RA:2701:C:H3' | 24:RA:2702:U:H5'' | 1.81 | 0.61 |
| 1:QA:266:G:O2' | 1:QA:267:C:OP2 | 2.16 | 0.61 |
| 1:QA:578:C:O2' | 1:QA:728:A:N3 | 2.29 | 0.61 |
| 2:QB:55:PHE:HA | 2:QB:58:ILE:HG12 | 1.83 | 0.61 |
| 24:RA:1011:G:OP1 | 39:RU:66:ASN:ND2 | 2.33 | 0.61 |
| 27:RE:78:LEU:HG | 27:RE:79:ARG:HD2 | 1.81 | 0.61 |
| 33:RO:80:ASP:OD2 | 38:RT:64:ARG:NH2 | 2.34 | 0.61 |
| 1:XA:152:A:H62 | 1:XA:169:C:N4 | 1.99 | 0.61 |
| 7:XG:16:LEU:HD11 | 9:XI:45:ALA:HB2 | 1.82 | 0.61 |
| 24:YA:574:C:N3 | 27:YE:145:LYS:NZ | 2.45 | 0.61 |
| 26:YD:146:GLU:HB2 | 26:YD:189:CYS:HB3 | 1.83 | 0.61 |
| 1:QA:1073:U:O2 | 2:QB:104:ASN:ND2 | 2.33 | 0.60 |
| 54:R9:25:VAL:HB | 54:R9:34:GLN:HB2 | 1.83 | 0.60 |
| 27:RE:2:LYS:HD3 | 27:RE:95:ILE:HG22 | 1.82 | 0.60 |
| 3:XC:17:ASP:O | 3:XC:54:ARG:NH2 | 2.34 | 0.60 |
| 6:XF:23:LYS:HA | 6:XF:26:ILE:HD12 | 1.83 | 0.60 |
| 22:XV:4:U:HO2' | 22:XV:5:G:H8 | 1.46 | 0.60 |
| 13:QM:22:ILE:N | 13:QM:22:ILE:HD12 | 2.15 | 0.60 |
| 26:RD:27:THR:HG21 | 26:RD:81:ALA:HB1 | 1.83 | 0.60 |
| 34:RP:106:LEU:HD21 | 34:RP:112:LEU:HD13 | 1.83 | 0.60 |
| 1:XA:1441:G:N2 | 1:XA:1460:A:H62 | 1.98 | 0.60 |
| 24:YA:380:U:H2' | 24:YA:381:G:H8 | 1.66 | 0.60 |
| 39:YU:90:VAL:HG22 | 40:YV:39:LEU:HD23 | 1.81 | 0.60 |
| 1:XA:272:C:H2' | 1:XA:273:A:H8 | 1.65 | 0.60 |
| 1:XA:736:C:H2' | 1:XA:737:A:H8 | 1.65 | 0.60 |
| 24:YA:1138:G:O2' | 32:YN:102:ALA:O | 2.19 | 0.60 |
| 24:RA:1288:U:O3' | 24:RA:1647:G:N2 | 2.34 | 0.60 |
| 24:RA:372:G:N2 | 24:RA:401:A:OP2 | 2.34 | 0.60 |
| 37:RS:30:ARG:HG2 | 37:RS:97:ARG:HH21 | 1.66 | 0.60 |
| 1:XA:1450:U:O2' | 1:XA:1451:A:N7 | 2.31 | 0.60 |
| 1:XA:736:C:H2' | 1:XA:737:A:C8 | 2.36 | 0.60 |
| 19:QS:41:VAL:HG13 | 19:QS:43:GLU:H | 1.64 | 0.60 |
| 24:RA:2030:A:H4' | 24:RA:2031:A:H8 | 1.67 | 0.60 |
| 24:RA:856:C:O2' | 24:RA:857:C:OP1 | 2.19 | 0.60 |
| 24:YA:857:C:OP2 | 45:Y0:77:ARG:NH2 | 2.34 | 0.60 |
| 24:YA:1418:G:N1 | 24:YA:1579:A:OP2 | 2.29 | 0.60 |
| 30:YH:149:ARG:NH2 | 30:YH:167:GLU:OE2 | 2.35 | 0.60 |
| 1:QA:1356:G:H2' | 1:QA:1357:A:C8 | 2.36 | 0.60 |
| 8:QH:112:LEU:HA | 8:QH:134:ILE:HG12 | 1.83 | 0.60 |
| 24:RA:2308:G:H22 | 24:RA:2311:A:H2 | 1.50 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:971:G:N2 | 1:XA:1363:A:OP2 | 2.34 | 0.60 |
| 1:XA:1414:U:H2' | 1:XA:1415:G:H8 | 1.67 | 0.60 |
| 29:YG:98:ARG:NH1 | 49:Y4:1:MET:SD | 2.74 | 0.60 |
| 24:YA:117:G:OP2 | 24:YA:119:A:O2' | 2.18 | 0.60 |
| 1:QA:272:C:H2' | 1:QA:273:A:H8 | 1.65 | 0.60 |
| 14:QN:45:ARG:O | 14:QN:49:HIS:ND1 | 2.32 | 0.60 |
| 1:QA:191(G):G:O2' | 20:QT:101:GLY:O | 2.19 | 0.60 |
| 50:R5:46:CYS:CB | 50:R5:49:CYS:SG | 2.89 | 0.60 |
| 24:RA:517:C:O2' | 41:RW:18:ARG:NH2 | 2.31 | 0.60 |
| 24:RA:527:C:C4 | 24:RA:2779:U:H5'' | 2.36 | 0.60 |
| 24:RA:583:G:OP2 | 39:RU:10:ARG:NH1 | 2.33 | 0.60 |
| 1:XA:1347:G:N2 | 1:XA:1374:A:OP2 | 2.35 | 0.60 |
| 1:XA:1500:A:H5'' | 1:XA:1508:G:H5'' | 1.84 | 0.60 |
| 3:XC:56:ASP:HB3 | 3:XC:67:THR:HB | 1.83 | 0.60 |
| 24:YA:26:G:H1' | 24:YA:515:A:H61 | 1.66 | 0.60 |
| 26:YD:147:LEU:HD12 | 26:YD:155:LEU:HD11 | 1.82 | 0.60 |
| 1:QA:123:C:OP1 | 1:QA:311:C:O2' | 2.20 | 0.60 |
| 24:RA:665:C:H2' | 24:RA:666:G:H8 | 1.67 | 0.60 |
| 30:RH:85:LYS:HD3 | 30:RH:86:GLU:H | 1.67 | 0.60 |
| 14:XN:39:LEU:HB2 | 14:XN:44:LEU:HD23 | 1.82 | 0.60 |
| 1:QA:1500:A:H5'' | 1:QA:1508:G:H5'' | 1.83 | 0.60 |
| 24:RA:1225:C:O2 | 40:RV:85:LYS:NZ | 2.32 | 0.60 |
| 24:RA:2068:U:H3 | 24:RA:2430:A:H2 | 1.49 | 0.60 |
| 24:YA:1365:A:O2' | 46:Y1:11:ARG:NH2 | 2.30 | 0.60 |
| 29:YG:29:TRP:O | 29:YG:33:ARG:NH1 | 2.34 | 0.60 |
| 1:QA:1376:U:OP1 | 7:QG:94:ARG:NH1 | 2.35 | 0.60 |
| 1:QA:673:G:H2' | 1:QA:674:G:C8 | 2.36 | 0.60 |
| 24:RA:1061:U:OP2 | 24:RA:1070:A:O2' | 2.15 | 0.60 |
| 4:XD:12:CYS:CB | 56:XD:301:SF4:S3 | 2.90 | 0.60 |
| 24:YA:770:G:OP1 | 52:Y7:8:ASN:ND2 | 2.32 | 0.60 |
| 3:QC:182:ILE:HD11 | 3:QC:201:TYR:HB3 | 1.83 | 0.59 |
| 1:QA:1312:G:H5' | 19:QS:5:LEU:HD11 | 1.84 | 0.59 |
| 24:RA:860:U:H2' | 24:RA:861:A:H8 | 1.67 | 0.59 |
| 24:RA:782:A:O2' | 26:RD:225:ALA:O | 2.19 | 0.59 |
| 38:RT:28:VAL:HG23 | 38:RT:88:ILE:HA | 1.82 | 0.59 |
| 41:RW:69:LEU:HD23 | 41:RW:107:LEU:HD13 | 1.84 | 0.59 |
| 1:XA:28:G:O2' | 1:XA:296:U:OP1 | 2.19 | 0.59 |
| 24:YA:1309:G:HO2' | 24:YA:1611:C:HO2' | 1.49 | 0.59 |
| 24:YA:2306:C:H3' | 24:YA:2307:G:H5'' | 1.83 | 0.59 |
| 24:YA:1657:C:H4' | 27:YE:133:LYS:HB3 | 1.84 | 0.59 |
| 18:QR:58:LEU:HD23 | 18:QR:62:GLU:HB3 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:RA:1967:C:H2' | 24:RA:1968:G:O4' | 2.03 | 0.59 |
| 24:RA:1030:G:OP2 | 35:RQ:128:LYS:NZ | 2.35 | 0.59 |
| 1:XA:643:C:H2' | 1:XA:644:G:H8 | 1.66 | 0.59 |
| 48:Y3:38:GLU:CD | 48:Y3:38:GLU:H | 2.03 | 0.59 |
| 24:YA:1967:C:H2' | 24:YA:1968:G:O4' | 2.02 | 0.59 |
| 30:YH:24:VAL:HG23 | 30:YH:35:VAL:HB | 1.83 | 0.59 |
| 45:R0:27:GLU:HG3 | 45:R0:68:GLU:HA | 1.85 | 0.59 |
| 30:RH:18:GLU:HB2 | 30:RH:25:LYS:HB3 | 1.84 | 0.59 |
| 4:XD:12:CYS:HB2 | 56:XD:301:SF4:S3 | 2.41 | 0.59 |
| 27:YE:9:VAL:HB | 27:YE:25:VAL:HG23 | 1.84 | 0.59 |
| 37:YS:10:ARG:NH1 | 37:YS:91:PRO:O | 2.35 | 0.59 |
| 13:QM:3:ARG:HA | 13:QM:9:ILE:HG21 | 1.83 | 0.59 |
| 1:QA:1304:G:OP1 | 21:QU:2:GLY:N | 2.35 | 0.59 |
| 24:RA:2328:A:H2' | 24:RA:2329:G:C8 | 2.37 | 0.59 |
| 31:RI:123:LEU:HD12 | 31:RI:142:VAL:HG23 | 1.83 | 0.59 |
| 1:XA:119:A:C8 | 1:XA:288:A:N1 | 2.70 | 0.59 |
| 1:XA:713:G:H2' | 1:XA:714:G:C8 | 2.36 | 0.59 |
| 1:XA:842:C:O2' | 1:XA:848:C:N4 | 2.35 | 0.59 |
| 42:YX:27:THR:HB | 42:YX:80:ILE:HG12 | 1.83 | 0.59 |
| 1:QA:1210:C:O2' | 1:QA:1213:A:O2' | 2.20 | 0.59 |
| 1:QA:790:A:OP1 | 22:QV:39:A:O2' | 2.19 | 0.59 |
| 1:QA:686:U:H1' | 11:QK:42:TRP:HE1 | 1.67 | 0.59 |
| 24:RA:662:G:OP1 | 34:RP:15:ARG:NH1 | 2.34 | 0.59 |
| 2:XB:132:LYS:HA | 2:XB:135:GLN:HB2 | 1.84 | 0.59 |
| 16:XP:6:LEU:HD12 | 16:XP:17:TYR:HB3 | 1.85 | 0.59 |
| 6:QF:100:ASN:ND2 | 18:QR:23:LYS:O | 2.27 | 0.59 |
| 24:RA:1363:C:O2' | 24:RA:1809:A:N3 | 2.33 | 0.59 |
| 24:RA:2576:G:O2' | 24:RA:2579:C:OP2 | 2.20 | 0.59 |
| 24:RA:2626:C:H2' | 24:RA:2627:G:H8 | 1.68 | 0.59 |
| 24:RA:956:G:OP2 | 35:RQ:14:ARG:NH2 | 2.35 | 0.59 |
| 24:YA:2471:C:H3' | 24:YA:2472:G:H8 | 1.68 | 0.59 |
| 24:YA:526:A:OP1 | 24:YA:527:C:OP1 | 2.20 | 0.59 |
| 7:QG:117:ALA:HA | 7:QG:120:ILE:HD12 | 1.85 | 0.59 |
| 24:RA:2893:G:H5'' | 24:RA:2894:G:H5' | 1.84 | 0.59 |
| 24:RA:764:A:H5' | 26:RD:210:GLY:HA2 | 1.84 | 0.59 |
| 26:RD:155:LEU:HD23 | 26:RD:177:LEU:HD11 | 1.84 | 0.59 |
| 35:RQ:41:TRP:HB3 | 35:RQ:94:VAL:HG11 | 1.85 | 0.59 |
| 1:XA:972:C:H4' | 10:XJ:57:LYS:HB2 | 1.84 | 0.59 |
| 24:YA:2123:G:H2' | 24:YA:2124:G:H8 | 1.68 | 0.59 |
| 24:YA:259:G:HO2' | 24:YA:621:A:HO2' | 1.46 | 0.59 |
| 48:R3:8:LEU:HG | 48:R3:28:LEU:HD13 | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:RH:45:VAL:HA | 30:RH:50:VAL:HG12 | 1.84 | 0.59 |
| 24:YA:1405:U:H2' | 24:YA:1406:U:H6 | 1.68 | 0.59 |
| 2:QB:32:ILE:HD11 | 2:QB:40:HIS:HB3 | 1.85 | 0.59 |
| 24:RA:2635:C:OP1 | 27:RE:78:LEU:HD13 | 2.03 | 0.59 |
| 27:YE:2:LYS:HE3 | 27:YE:95:ILE:HG22 | 1.84 | 0.59 |
| 37:YS:110:LEU:HD12 | 37:YS:112:PHE:H | 1.68 | 0.59 |
| 1:QA:1321:C:H5'' | 1:QA:1322:C:H5'' | 1.85 | 0.59 |
| 1:QA:689:C:OP1 | 11:QK:44:SER:OG | 2.15 | 0.59 |
| 1:QA:827:U:O2 | 1:QA:874:G:N2 | 2.36 | 0.59 |
| 6:QF:47:ARG:HH22 | 6:QF:56:PRO:HB2 | 1.68 | 0.59 |
| 20:QT:53:LEU:HD23 | 20:QT:100:ILE:HG23 | 1.84 | 0.59 |
| 24:RA:577:G:O2' | 24:RA:1254:A:OP1 | 2.21 | 0.59 |
| 24:RA:1754:C:OP1 | 38:RT:96:ARG:NH1 | 2.36 | 0.59 |
| 31:RI:14:ASP:O | 31:RI:16:GLY:N | 2.36 | 0.59 |
| 1:XA:1209:C:O2' | 1:XA:1214:C:N4 | 2.35 | 0.59 |
| 14:YN:27:CYS:SG | 14:YN:40:CYS:HB3 | 2.43 | 0.59 |
| 16:XP:6:LEU:HB3 | 16:XP:17:TYR:HD1 | 1.67 | 0.59 |
| 24:YA:1012:U:O2' | 24:YA:1013:C:P | 2.61 | 0.59 |
| 24:YA:840:C:H2' | 24:YA:841:A:H8 | 1.68 | 0.59 |
| 25:YB:44:G:O2' | 25:YB:47:C:N4 | 2.34 | 0.59 |
| 1:QA:1422:G:H5'' | 33:RO:48:PRO:HB3 | 1.84 | 0.58 |
| 4:QD:15:GLU:HG2 | 4:QD:63:LYS:HD3 | 1.85 | 0.58 |
| 7:QG:67:GLU:HA | 7:QG:70:LYS:HD3 | 1.84 | 0.58 |
| 13:QM:25:ILE:CD1 | 13:QM:66:LEU:HD11 | 2.33 | 0.58 |
| 1:XA:1095:U:OP2 | 1:XA:1108:G:N1 | 2.36 | 0.58 |
| 1:XA:514:C:H2' | 1:XA:515:G:H8 | 1.68 | 0.58 |
| 24:YA:987:G:O2' | 24:YA:1000:A:N3 | 2.34 | 0.58 |
| 33:YO:107:ARG:NH1 | 38:YT:36:GLU:OE2 | 2.36 | 0.58 |
| 24:RA:1212:G:N2 | 24:RA:1236:G:O2' | 2.33 | 0.58 |
| 24:RA:2323:G:H1 | 24:RA:2332:U:H3 | 1.50 | 0.58 |
| 1:XA:486:U:H2' | 1:XA:487:A:H8 | 1.67 | 0.58 |
| 24:YA:483:A:O2' | 43:YY:49:VAL:O | 2.16 | 0.58 |
| 1:QA:1085:U:OP1 | 1:QA:1094:G:N2 | 2.36 | 0.58 |
| 7:QG:116:ALA:HA | 7:QG:119:ARG:HE | 1.68 | 0.58 |
| 50:R5:36:CYS:HB3 | 50:R5:49:CYS:HB3 | 1.85 | 0.58 |
| 24:RA:2119:A:N6 | 24:RA:2170:A:N7 | 2.50 | 0.58 |
| 37:RS:10:ARG:NH1 | 37:RS:91:PRO:O | 2.37 | 0.58 |
| 24:YA:2314:C:H2' | 24:YA:2315:G:H8 | 1.68 | 0.58 |
| 24:YA:2718:G:O2' | 24:YA:2847:U:OP1 | 2.20 | 0.58 |
| 24:YA:321:G:O2' | 24:YA:340:A:N3 | 2.36 | 0.58 |
| 1:QA:1266:G:N2 | 1:QA:1269:A:OP2 | 2.27 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:QD:100:ARG:NH2 | 4:QD:136:PRO:O | 2.36 | 0.58 |
| 24:RA:2008:C:H2' | 24:RA:2009:G:H8 | 1.68 | 0.58 |
| 34:RP:68:GLN:HG2 | 53:R8:12:LYS:HG2 | 1.85 | 0.58 |
| 1:XA:426:G:OP1 | 4:XD:38:TYR:OH | 2.17 | 0.58 |
| 6:XF:80:ARG:HE | 6:XF:88:VAL:HB | 1.69 | 0.58 |
| 1:XA:243:A:H4' | 1:XA:244:U:O5' | 2.02 | 0.58 |
| 1:XA:34:C:H2' | 1:XA:35:G:H8 | 1.69 | 0.58 |
| 2:XB:80:ILE:HD13 | 2:XB:212:GLN:HB2 | 1.86 | 0.58 |
| 1:QA:1502:A:H2 | 1:QA:1505:G:H1 | 1.52 | 0.58 |
| 6:QF:14:LEU:HD11 | 6:QF:18:GLN:HB2 | 1.84 | 0.58 |
| 1:XA:1147:C:HO2' | 9:XI:5:TYR:HH | 1.50 | 0.58 |
| 1:XA:954:G:H21 | 1:XA:1227:A:H62 | 1.50 | 0.58 |
| 12:XL:37:CYS:HA | 12:XL:58:VAL:HA | 1.86 | 0.58 |
| 1:QA:189:U:O2 | 17:QQ:63:ARG:NH2 | 2.36 | 0.58 |
| 6:QF:23:LYS:HA | 6:QF:26:ILE:HD12 | 1.85 | 0.58 |
| 46:R1:65:SER:HG | 46:R1:66:HIS:HD1 | 1.51 | 0.58 |
| 24:RA:1798:U:O2' | 24:RA:1802:A:N3 | 2.36 | 0.58 |
| 24:RA:299:A:N3 | 24:RA:319:C:O2' | 2.35 | 0.58 |
| 44:RZ:52:SER:O | 44:RZ:54:HIS:ND1 | 2.34 | 0.58 |
| 1:XA:855:G:OP2 | 1:XA:871:U:N3 | 2.37 | 0.58 |
| 1:QA:34:C:H2' | 1:QA:35:G:H8 | 1.69 | 0.58 |
| 24:RA:2328:A:H2' | 24:RA:2329:G:H8 | 1.68 | 0.58 |
| 1:QA:1432:G:OP1 | 38:RT:108:ARG:N | 2.37 | 0.58 |
| 24:YA:1062:G:N2 | 24:YA:1077:A:N1 | 2.51 | 0.58 |
| 24:YA:1818:U:OP2 | 26:YD:157:ARG:NE | 2.36 | 0.58 |
| 26:YD:143:HIS:ND1 | 26:YD:194:GLY:O | 2.31 | 0.58 |
| 1:QA:407:G:H5'' | 4:QD:115:ARG:HD3 | 1.85 | 0.58 |
| 1:QA:7:G:H5' | 1:QA:298:A:O4' | 2.03 | 0.58 |
| 53:R8:29:LYS:O | 53:R8:31:HIS:N | 2.37 | 0.58 |
| 24:RA:414:C:O2 | 24:RA:1864:U:O2' | 2.22 | 0.58 |
| 24:RA:300:A:OP1 | 43:RY:86:ARG:NH2 | 2.36 | 0.58 |
| 14:YN:57:ARG:HH21 | 14:YN:58:LYS:HG2 | 1.69 | 0.58 |
| 1:XA:1455:G:H5'' | 20:XT:31:SER:HB2 | 1.86 | 0.58 |
| 24:YA:2151:G:H2' | 24:YA:2152:G:H8 | 1.69 | 0.58 |
| 24:YA:2213:U:O2 | 46:Y1:52:ARG:NH2 | 2.37 | 0.58 |
| 24:YA:2328:A:H2' | 24:YA:2329:G:H8 | 1.69 | 0.58 |
| 24:YA:2642:G:H5' | 32:YN:78:TYR:CD2 | 2.39 | 0.58 |
| 26:YD:148:GLU:HB2 | 26:YD:151:LYS:HD2 | 1.86 | 0.58 |
| 24:YA:1902:C:OP1 | 26:YD:242:ARG:NH1 | 2.37 | 0.58 |
| 27:YE:201:THR:HG22 | 27:YE:203:LYS:H | 1.68 | 0.58 |
| 7:QG:45:ASP:OD2 | 7:QG:115:ARG:NH2 | 2.37 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:RA:1272:A:OP2 | 24:RA:1647:G:OP1 | 2.21 | 0.58 |
| 24:RA:630:G:OP1 | 53:R8:46:ARG:NH1 | 2.37 | 0.58 |
| 8:XH:109:ILE:HD11 | 8:XH:120:THR:HB | 1.85 | 0.58 |
| 50:Y5:16:ARG:NH1 | 50:Y5:17:ASP:OD1 | 2.37 | 0.58 |
| 24:YA:2747:G:H21 | 24:YA:2757:A:H62 | 1.52 | 0.58 |
| 24:YA:83:G:H1 | 24:YA:102:G:HO2' | 1.51 | 0.58 |
| 28:YF:134:GLY:H | 28:YF:162:LEU:HD12 | 1.69 | 0.58 |
| 33:YO:80:ASP:OD2 | 38:YT:64:ARG:NH2 | 2.37 | 0.58 |
| 1:QA:376:G:H5'' | 16:QP:5:ARG:HB2 | 1.85 | 0.57 |
| 47:R2:10:LEU:HD21 | 47:R2:14:ARG:HH21 | 1.69 | 0.57 |
| 24:RA:521:G:H2' | 24:RA:522:G:H8 | 1.69 | 0.57 |
| 26:RD:142:VAL:HG23 | 26:RD:193:VAL:HA | 1.86 | 0.57 |
| 38:RT:123:GLN:O | 38:RT:125:ARG:N | 2.37 | 0.57 |
| 24:YA:955:C:OP1 | 35:YQ:85:LYS:NZ | 2.32 | 0.57 |
| 1:QA:1080:A:H5' | 5:QE:16:THR:HG21 | 1.85 | 0.57 |
| 1:QA:816:A:OP1 | 1:QA:1526:G:O2' | 2.21 | 0.57 |
| 13:QM:14:ARG:NH2 | 13:QM:16:ASP:OD2 | 2.37 | 0.57 |
| 24:RA:593:G:H4' | 53:R8:61:LEU:HD13 | 1.86 | 0.57 |
| 24:RA:345:A:H2' | 24:RA:347:A:H62 | 1.70 | 0.57 |
| 1:XA:1510:U:H2' | 1:XA:1511:G:C8 | 2.40 | 0.57 |
| 1:XA:31:G:O2' | 1:XA:48:C:N4 | 2.36 | 0.57 |
| 1:XA:78:G:O2' | 1:XA:79:G:OP1 | 2.20 | 0.57 |
| 50:Y5:41:PRO:O | 50:Y5:44:THR:OG1 | 2.21 | 0.57 |
| 50:Y5:36:CYS:HB3 | 50:Y5:49:CYS:HB3 | 1.85 | 0.57 |
| 24:YA:1109:C:O2' | 24:YA:1110:G:OP1 | 2.21 | 0.57 |
| 24:YA:2705:A:O2' | 24:YA:2852:G:OP1 | 2.16 | 0.57 |
| 24:YA:510:C:C2' | 24:YA:511:U:H5' | 2.34 | 0.57 |
| 27:YE:16:ARG:NH2 | 27:YE:171:GLU:OE2 | 2.37 | 0.57 |
| 1:QA:738:C:OP1 | 6:QF:2:ARG:NH1 | 2.37 | 0.57 |
| 24:RA:65:C:H1' | 24:RA:456:C:H42 | 1.68 | 0.57 |
| 29:RG:114:ILE:HA | 29:RG:136:ARG:HH22 | 1.69 | 0.57 |
| 32:RN:34:LEU:HD12 | 32:RN:107:LEU:HD11 | 1.86 | 0.57 |
| 1:XA:1264:C:H2' | 1:XA:1265:G:H8 | 1.69 | 0.57 |
| 6:XF:94:GLN:OE1 | 18:XR:32:ARG:NH1 | 2.37 | 0.57 |
| 14:XM:27:CYS:HB3 | 14:XM:43:CYS:SG | 2.43 | 0.57 |
| 11:QK:86:GLY:O | 11:QK:91:ARG:NH1 | 2.38 | 0.57 |
| 48:R3:15:TYR:O | 48:R3:20:LYS:NZ | 2.38 | 0.57 |
| 24:RA:1600:C:H2' | 24:RA:1601:G:H8 | 1.68 | 0.57 |
| 24:RA:321:G:O2' | 24:RA:340:A:N3 | 2.36 | 0.57 |
| 38:RT:132:LYS:O | 38:RT:136:GLN:NE2 | 2.37 | 0.57 |
| 1:XA:1224:G:H21 | 13:XM:102:ARG:HH22 | 1.52 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:YA:2329:G:H2' | 24:YA:2330:G:H8 | 1.68 | 0.57 |
| 24:RA:1059:G:O6 | 24:RA:1079:C:N4 | 2.37 | 0.57 |
| 41:RW:24:ILE:HA | 41:RW:27:LYS:HD2 | 1.85 | 0.57 |
| 2:XB:55:PHE:HA | 2:XB:58:ILE:HG12 | 1.87 | 0.57 |
| 48:Y3:15:TYR:O | 48:Y3:20:LYS:NZ | 2.37 | 0.57 |
| 24:YA:193:U:N3 | 24:YA:203:C:O2 | 2.38 | 0.57 |
| 1:QA:235:C:H2' | 1:QA:236:G:H8 | 1.70 | 0.57 |
| 24:RA:1043:C:H42 | 24:RA:1112:G:H1 | 1.51 | 0.57 |
| 24:RA:958:U:OP2 | 35:RQ:14:ARG:NH1 | 2.37 | 0.57 |
| 24:YA:2140:C:H2' | 24:YA:2141:G:H8 | 1.67 | 0.57 |
| 24:YA:2626:C:H2' | 24:YA:2627:G:H8 | 1.70 | 0.57 |
| 24:YA:604:G:OP2 | 34:YP:90:ARG:NH1 | 2.37 | 0.57 |
| 24:YA:662:G:OP1 | 34:YP:15:ARG:NH1 | 2.38 | 0.57 |
| 24:YA:814:C:H41 | 34:YP:25:SER:HA | 1.70 | 0.57 |
| 1:QA:684:A:O2' | 11:QK:39:PRO:O | 2.20 | 0.57 |
| 3:QC:14:ILE:HG12 | 3:QC:15:THR:HG23 | 1.86 | 0.57 |
| 24:RA:2047:U:H2' | 24:RA:2048:G:H8 | 1.70 | 0.57 |
| 24:RA:627:A:H4' | 24:RA:628:G:H5' | 1.86 | 0.57 |
| 24:RA:834:C:H2' | 24:RA:835:A:H8 | 1.70 | 0.57 |
| 24:RA:2547:U:O2 | 33:RO:23:ARG:NH2 | 2.38 | 0.57 |
| 1:XA:1356:G:H2' | 1:XA:1357:A:H8 | 1.68 | 0.57 |
| 1:XA:565:U:H5'' | 1:XA:566:G:H2' | 1.87 | 0.57 |
| 24:YA:2329:G:H2' | 24:YA:2330:G:C8 | 2.40 | 0.57 |
| 24:YA:277:C:H5'' | 24:YA:278:A:H5' | 1.85 | 0.57 |
| 24:YA:2867:G:O2' | 24:YA:2868:A:H8 | 1.88 | 0.57 |
| 24:YA:2635:C:O2' | 27:YE:80:GLU:OE2 | 2.20 | 0.57 |
| 1:QA:1186:G:H2' | 9:QI:111:ARG:HH22 | 1.69 | 0.57 |
| 1:QA:770:C:H2' | 1:QA:771:G:H8 | 1.69 | 0.57 |
| 2:QB:78:GLN:O | 2:QB:94:ASN:ND2 | 2.36 | 0.57 |
| 3:QC:19:GLU:HG2 | 3:QC:40:ARG:HH21 | 1.69 | 0.57 |
| 45:R0:25:ARG:HB2 | 45:R0:37:LEU:HD13 | 1.86 | 0.57 |
| 24:RA:1262:A:OP1 | 41:RW:99:ARG:NH1 | 2.34 | 0.57 |
| 44:RZ:10:ARG:NH2 | 44:RZ:37:VAL:O | 2.37 | 0.57 |
| 1:XA:973:G:H3' | 1:XA:974:A:H5'' | 1.85 | 0.57 |
| 24:YA:1833:U:O2' | 24:YA:1969:A:N1 | 2.34 | 0.57 |
| 28:YF:116:ASP:OD1 | 28:YF:119:ARG:NH2 | 2.37 | 0.57 |
| 39:YU:92:ARG:HD2 | 40:YV:11:GLN:HB2 | 1.87 | 0.57 |
| 44:YZ:52:SER:O | 44:YZ:54:HIS:ND1 | 2.38 | 0.57 |
| 1:QA:1172:C:H2' | 1:QA:1173:G:H8 | 1.70 | 0.57 |
| 1:QA:298:A:H8 | 1:QA:298:A:OP1 | 1.88 | 0.57 |
| 1:QA:1298:C:OP2 | 7:QG:114:ARG:NH1 | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1296:C:OP1 | 13:QM:44:ARG:NH2 | 2.38 | 0.57 |
| 1:XA:107:G:OP1 | 1:XA:325:A:N6 | 2.38 | 0.57 |
| 3:XC:150:LYS:HE3 | 3:XC:167:TRP:HE1 | 1.70 | 0.57 |
| 1:XA:599:C:O2' | 8:XH:129:VAL:O | 2.18 | 0.57 |
| 24:YA:1353:A:OP2 | 24:YA:1377:G:N1 | 2.30 | 0.57 |
| 24:YA:775:G:H4' | 24:YA:776:G:H5' | 1.86 | 0.57 |
| 24:YA:782:A:O2' | 26:YD:225:ALA:O | 2.22 | 0.57 |
| 32:YN:34:LEU:O | 32:YN:49:GLY:HA3 | 2.04 | 0.57 |
| 38:YT:29:ARG:HB2 | 38:YT:46:GLU:HG3 | 1.87 | 0.57 |
| 1:QA:715:A:H2' | 1:QA:716:A:C8 | 2.39 | 0.57 |
| 3:QC:11:ARG:NH2 | 3:QC:177:THR:O | 2.38 | 0.57 |
| 3:QC:58:GLU:HB2 | 3:QC:65:ALA:HB3 | 1.86 | 0.57 |
| 1:XA:522:C:H41 | 12:XL:53:ARG:HH22 | 1.51 | 0.57 |
| 25:YB:33:G:H5' | 29:YG:2:PRO:HG3 | 1.87 | 0.57 |
| 24:YA:2495:G:H5'' | 35:YQ:81:VAL:HG12 | 1.87 | 0.57 |
| 42:YX:36:LYS:NZ | 42:YX:54:VAL:O | 2.34 | 0.57 |
| 1:QA:235:C:O2 | 17:QQ:4:LYS:NZ | 2.33 | 0.56 |
| 24:RA:275:G:H3' | 24:RA:276:A:H5'' | 1.87 | 0.56 |
| 26:RD:108:PRO:HA | 26:RD:196:VAL:HA | 1.86 | 0.56 |
| 1:XA:1321:C:H5'' | 1:XA:1322:C:H2' | 1.86 | 0.56 |
| 2:XB:82:ARG:NH1 | 2:XB:92:TYR:OH | 2.38 | 0.56 |
| 24:YA:144:C:H2' | 24:YA:145:G:H8 | 1.70 | 0.56 |
| 1:QA:1053:G:H5' | 1:QA:1054:C:H5' | 1.85 | 0.56 |
| 13:QM:108:ARG:HE | 13:QM:114:ARG:HD2 | 1.69 | 0.56 |
| 24:RA:2232:U:OP2 | 46:R1:40:ARG:NH2 | 2.37 | 0.56 |
| 24:RA:815:C:OP2 | 40:RV:83:ARG:NH1 | 2.39 | 0.56 |
| 25:RB:52:A:HO2' | 25:RB:53:A:H8 | 1.53 | 0.56 |
| 25:RB:22:U:H3 | 25:RB:61:G:H1 | 1.52 | 0.56 |
| 27:RE:52:LEU:O | 27:RE:74:PRO:HA | 2.05 | 0.56 |
| 32:RN:34:LEU:HD11 | 32:RN:120:LEU:HD12 | 1.88 | 0.56 |
| 34:RP:47:ASP:OD2 | 34:RP:50:ARG:NH2 | 2.38 | 0.56 |
| 1:XA:401:C:O2' | 1:XA:621:A:N3 | 2.37 | 0.56 |
| 53:Y8:33:ASN:HA | 53:Y8:36:LYS:HD2 | 1.85 | 0.56 |
| 24:YA:814:C:H1' | 24:YA:1226:G:H21 | 1.70 | 0.56 |
| 24:YA:1315:C:O2' | 24:YA:1392:A:N3 | 2.35 | 0.56 |
| 24:YA:2030:A:H4' | 24:YA:2031:A:H8 | 1.69 | 0.56 |
| 19:QS:22:LEU:HD21 | 19:QS:28:LYS:HA | 1.87 | 0.56 |
| 46:R1:52:ARG:NH2 | 46:R1:55:GLY:O | 2.37 | 0.56 |
| 24:RA:2848:G:O2' | 24:RA:2867:G:N2 | 2.37 | 0.56 |
| 35:RQ:134:ARG:NH1 | 44:RZ:119:GLU:OE2 | 2.38 | 0.56 |
| 44:RZ:4:ARG:HB3 | 44:RZ:60:GLU:HG3 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:XC:153:VAL:HB | 3:XC:196:LEU:HD21 | 1.87 | 0.56 |
| 1:XA:933:G:O6 | 7:XG:3:ARG:NH2 | 2.38 | 0.56 |
| 10:XJ:51:ARG:O | 14:XN:45:ARG:NH1 | 2.38 | 0.56 |
| 24:YA:447:A:H4' | 24:YA:449:A:N7 | 2.20 | 0.56 |
| 1:XA:992:U:O4 | 1:XA:1044:A:N7 | 2.39 | 0.56 |
| 4:XD:61:LYS:HG2 | 4:XD:61:LYS:NZ | 2.21 | 0.56 |
| 1:XA:1368:G:OP1 | 9:XI:111:ARG:NH2 | 2.37 | 0.56 |
| 9:XI:9:ARG:H | 9:XI:79:LEU:HD23 | 1.69 | 0.56 |
| 24:YA:1354:A:H3' | 24:YA:1355:G:H8 | 1.71 | 0.56 |
| 24:YA:2023:G:H5' | 24:YA:2617:C:H4' | 1.87 | 0.56 |
| 24:YA:467:G:N7 | 52:Y7:39:ARG:NH2 | 2.54 | 0.56 |
| 9:QI:28:VAL:HG12 | 9:QI:63:ILE:HB | 1.87 | 0.56 |
| 19:QS:3:ARG:HH22 | 19:QS:7:LYS:HB2 | 1.70 | 0.56 |
| 24:RA:1171:G:N7 | 24:RA:1174:A:N6 | 2.52 | 0.56 |
| 24:RA:2696:U:H2' | 24:RA:2697:G:C8 | 2.41 | 0.56 |
| 24:YA:1592:C:H2' | 24:YA:1593:G:H8 | 1.71 | 0.56 |
| 1:QA:191(F):U:H2' | 1:QA:191(G):G:H8 | 1.70 | 0.56 |
| 1:QA:713:G:H2' | 1:QA:714:G:C8 | 2.41 | 0.56 |
| 19:QS:50:ALA:HB1 | 19:QS:57:HIS:HB3 | 1.87 | 0.56 |
| 24:RA:1689:A:H62 | 24:RA:1698:A:H2 | 1.53 | 0.56 |
| 1:XA:501:C:H2' | 1:XA:502:G:H8 | 1.71 | 0.56 |
| 7:XG:150:ALA:HB1 | 11:XK:57:THR:HG21 | 1.87 | 0.56 |
| 24:YA:1062:G:H1 | 24:YA:1076:C:H42 | 1.54 | 0.56 |
| 24:YA:297:C:OP1 | 43:YY:87:LYS:NZ | 2.31 | 0.56 |
| 24:YA:589:C:H2' | 24:YA:590:A:C8 | 2.41 | 0.56 |
| 24:RA:2680:C:H5' | 27:RE:189:PRO:HA | 1.86 | 0.56 |
| 1:XA:143:A:H2 | 1:XA:220:G:H1 | 1.53 | 0.56 |
| 1:XA:414:A:OP2 | 1:XA:428:G:N2 | 2.36 | 0.56 |
| 43:YY:29:GLU:HB3 | 43:YY:38:ILE:HD12 | 1.86 | 0.56 |
| 1:QA:1230:C:H5' | 22:QV:31:C:H5'' | 1.88 | 0.56 |
| 6:QF:9:VAL:HB | 6:QF:87:ARG:HB2 | 1.87 | 0.56 |
| 30:RH:40:GLU:HA | 30:RH:42:ARG:HH12 | 1.70 | 0.56 |
| 1:XA:1077:G:N2 | 1:XA:1080:A:OP2 | 2.28 | 0.56 |
| 1:XA:953:G:H5' | 1:XA:965:A:H61 | 1.70 | 0.56 |
| 4:XD:182:LYS:HD3 | 4:XD:184:LYS:HE3 | 1.88 | 0.56 |
| 24:YA:581:C:H2' | 24:YA:582:G:H8 | 1.71 | 0.56 |
| 24:YA:851:U:H2' | 24:YA:852:G:H8 | 1.71 | 0.56 |
| 1:QA:739:C:O2' | 15:QO:42:HIS:ND1 | 2.37 | 0.56 |
| 22:XV:44:G:H2' | 22:XV:45:G:C8 | 2.41 | 0.56 |
| 24:YA:1056:G:H4' | 24:YA:1086:A:H8 | 1.70 | 0.56 |
| 24:YA:2701:C:H3' | 24:YA:2702:U:C5' | 2.32 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:YA:310:A:O2' | 24:YA:311:A:OP2 | 2.17 | 0.56 |
| 1:QA:376:G:H1 | 1:QA:387:U:H3 | 1.53 | 0.56 |
| 1:QA:401:C:O2' | 1:QA:621:A:N3 | 2.36 | 0.56 |
| 24:RA:503:A:H4' | 24:RA:504:U:H5' | 1.88 | 0.56 |
| 2:XB:87:ARG:NH1 | 2:XB:220:ASP:OD1 | 2.36 | 0.56 |
| 14:YN:24:CYS:HB2 | 14:YN:28:GLY:H | 1.71 | 0.56 |
| 28:YF:116:ASP:OD2 | 34:YP:1:MET:N | 2.37 | 0.56 |
| 24:RA:1869:G:H5' | 24:RA:1870:C:OP2 | 2.05 | 0.56 |
| 24:RA:301:G:OP2 | 43:RY:84:ARG:NH2 | 2.38 | 0.56 |
| 24:RA:558:G:H2' | 24:RA:559:G:H8 | 1.71 | 0.56 |
| 1:XA:21:G:H2' | 1:XA:22:G:C8 | 2.41 | 0.56 |
| 24:YA:259:G:O2' | 24:YA:621:A:O2' | 2.20 | 0.56 |
| 24:YA:665:C:H2' | 24:YA:666:G:H8 | 1.70 | 0.56 |
| 1:QA:945:G:N2 | 1:QA:1334:G:O2' | 2.38 | 0.55 |
| 7:QG:29:LYS:HE2 | 7:QG:105:VAL:HB | 1.88 | 0.55 |
| 23:QX:6:C:H2' | 23:QX:7:A:H8 | 1.71 | 0.55 |
| 24:RA:1226:G:OP1 | 40:RV:69:LYS:NZ | 2.33 | 0.55 |
| 24:RA:1853:A:N3 | 24:RA:2233:U:O2' | 2.35 | 0.55 |
| 24:RA:576:U:H2' | 24:RA:577:G:C8 | 2.41 | 0.55 |
| 1:XA:1498:U:OP2 | 23:XX:16:C:O2' | 2.20 | 0.55 |
| 1:XA:811:C:O2' | 1:XA:901:A:N1 | 2.39 | 0.55 |
| 24:YA:2336:A:H61 | 45:Y0:43:THR:HG21 | 1.70 | 0.55 |
| 24:YA:2636:U:H3 | 24:YA:2782:G:H1 | 1.54 | 0.55 |
| 35:YQ:31:ASP:OD1 | 35:YQ:134:ARG:NH1 | 2.39 | 0.55 |
| 38:YT:132:LYS:O | 38:YT:136:GLN:NE2 | 2.39 | 0.55 |
| 1:QA:1124:G:H1' | 10:QJ:38:ILE:HD13 | 1.88 | 0.55 |
| 1:QA:114:U:H2' | 1:QA:115:G:C8 | 2.41 | 0.55 |
| 1:QA:483:C:OP2 | 1:QA:484:G:O2' | 2.17 | 0.55 |
| 24:RA:1509:C:H3' | 24:RA:1510:A:C5' | 2.36 | 0.55 |
| 24:RA:743:G:O2' | 24:RA:1659:U:OP1 | 2.19 | 0.55 |
| 27:RE:104:VAL:HG22 | 27:RE:198:VAL:HG12 | 1.87 | 0.55 |
| 33:RO:107:ARG:NH1 | 38:RT:36:GLU:OE2 | 2.37 | 0.55 |
| 44:RZ:27:VAL:HG22 | 44:RZ:85:HIS:HE1 | 1.71 | 0.55 |
| 1:XA:662:G:H2' | 1:XA:663:A:C8 | 2.40 | 0.55 |
| 8:XH:33:GLU:OE1 | 8:XH:50:ARG:NH1 | 2.38 | 0.55 |
| 1:QA:1071:C:H2' | 1:QA:1072:G:H8 | 1.71 | 0.55 |
| 1:QA:501:C:H2' | 1:QA:502:G:H8 | 1.70 | 0.55 |
| 1:QA:958:A:N3 | 1:QA:985:C:O2' | 2.33 | 0.55 |
| 34:RP:52:GLU:OE2 | 53:R8:52:LYS:NZ | 2.39 | 0.55 |
| 24:YA:251:A:OP1 | 53:Y8:7:HIS:NE2 | 2.37 | 0.55 |
| 24:YA:24:G:O2' | 41:YW:78:GLU:O | 2.25 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:YD:155:LEU:HD23 | 26:YD:177:LEU:HD11 | 1.87 | 0.55 |
| 1:QA:243:A:H4' | 1:QA:244:U:O5' | 2.06 | 0.55 |
| 8:QH:41:ARG:NH2 | 8:QH:123:GLU:OE2 | 2.40 | 0.55 |
| 24:RA:2010:G:H5'' | 41:RW:42:ARG:HB2 | 1.87 | 0.55 |
| 24:RA:518:G:O5' | 41:RW:18:ARG:NH1 | 2.39 | 0.55 |
| 1:XA:1310:G:O2' | 1:XA:1311:G:OP1 | 2.23 | 0.55 |
| 1:XA:152:A:H62 | 1:XA:169:C:H42 | 1.53 | 0.55 |
| 1:XA:946:A:H2' | 1:XA:947:G:C8 | 2.41 | 0.55 |
| 7:XG:5:ARG:HD3 | 7:XG:7:ALA:H | 1.70 | 0.55 |
| 50:Y5:36:CYS:O | 50:Y5:37:LYS:HB3 | 2.06 | 0.55 |
| 24:YA:1639:U:H2' | 24:YA:1640:C:H5'' | 1.89 | 0.55 |
| 24:YA:679:C:H2' | 24:YA:680:G:H8 | 1.71 | 0.55 |
| 24:YA:706:A:OP1 | 26:YD:7:LYS:NZ | 2.29 | 0.55 |
| 36:YR:86:ARG:NH2 | 36:YR:118:GLU:OXT | 2.40 | 0.55 |
| 1:QA:1095:U:OP1 | 1:QA:1108:G:N2 | 2.32 | 0.55 |
| 1:QA:1104:G:H4' | 2:QB:111:ARG:CZ | 2.36 | 0.55 |
| 1:QA:946:A:H2' | 1:QA:947:G:C8 | 2.42 | 0.55 |
| 12:QL:60:LEU:HD12 | 12:QL:62:SER:H | 1.71 | 0.55 |
| 13:QM:106:ASN:N | 13:QM:106:ASN:OD1 | 2.37 | 0.55 |
| 50:R5:46:CYS:SG | 50:R5:49:CYS:N | 2.78 | 0.55 |
| 24:RA:1359:A:H62 | 24:RA:1372:U:H3 | 1.54 | 0.55 |
| 24:RA:1422:G:H1 | 24:RA:1576:U:H3 | 1.52 | 0.55 |
| 24:RA:949:C:H2' | 24:RA:950:G:H8 | 1.72 | 0.55 |
| 31:RI:54:GLN:OE1 | 31:RI:57:ARG:NH2 | 2.39 | 0.55 |
| 39:RU:91:ASP:O | 39:RU:93:LYS:N | 2.39 | 0.55 |
| 35:RQ:62:GLY:HA2 | 44:RZ:116:VAL:HG21 | 1.89 | 0.55 |
| 47:Y2:4:SER:OG | 47:Y2:5:GLU:N | 2.40 | 0.55 |
| 24:YA:1971:A:OP2 | 26:YD:242:ARG:NH2 | 2.34 | 0.55 |
| 24:YA:2809:A:H2' | 24:YA:2810:A:C8 | 2.42 | 0.55 |
| 24:YA:2052:G:H4' | 27:YE:143:ASN:O | 2.06 | 0.55 |
| 24:RA:1639:U:H2' | 24:RA:1640:C:H5'' | 1.89 | 0.55 |
| 24:RA:2070:G:H2' | 24:RA:2071:A:H8 | 1.72 | 0.55 |
| 9:XI:82:ALA:HB1 | 9:XI:102:LEU:HD22 | 1.88 | 0.55 |
| 24:YA:2124:G:H3' | 24:YA:2125:G:H8 | 1.71 | 0.55 |
| 10:QJ:21:GLN:HA | 10:QJ:24:VAL:HG12 | 1.89 | 0.55 |
| 1:QA:581:G:O3' | 15:QO:64:ARG:NH2 | 2.40 | 0.55 |
| 24:RA:1359:A:N6 | 24:RA:1372:U:H3 | 2.05 | 0.55 |
| 24:RA:1804:C:N4 | 24:RA:1814:G:N2 | 2.55 | 0.55 |
| 24:RA:2030:A:H4' | 24:RA:2031:A:C8 | 2.42 | 0.55 |
| 25:RB:44:G:O2' | 25:RB:47:C:N4 | 2.38 | 0.55 |
| 33:RO:23:ARG:NH2 | 33:RO:28:SER:O | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:XA:359:U:H3' | 1:XA:360:A:H8 | 1.72 | 0.55 |
| 23:XX:5:A:H2' | 23:XX:6:G:H8 | 1.72 | 0.55 |
| 33:YO:43:VAL:HG23 | 33:YO:55:GLY:H | 1.72 | 0.55 |
| 43:YY:79:CYS:HB3 | 43:YY:102:CYS:HB3 | 1.88 | 0.55 |
| 24:RA:1019:U:H3 | 24:RA:1142(A):A:H62 | 1.55 | 0.55 |
| 24:RA:182:A:N3 | 24:RA:433:C:O2' | 2.37 | 0.55 |
| 24:RA:2375:G:N2 | 24:RA:2378:A:OP2 | 2.36 | 0.55 |
| 24:RA:442:G:H1' | 28:RF:48:THR:HG21 | 1.89 | 0.55 |
| 3:XC:6:HIS:HE1 | 3:XC:8:ILE:HB | 1.72 | 0.55 |
| 7:XG:16:LEU:HD22 | 9:XI:44:VAL:HG13 | 1.89 | 0.55 |
| 1:XA:35:G:O2' | 12:XL:118:SER:O | 2.19 | 0.55 |
| 18:XR:56:THR:HG23 | 18:XR:58:LEU:H | 1.72 | 0.55 |
| 24:YA:431:U:H2' | 24:YA:432:A:H8 | 1.72 | 0.55 |
| 24:YA:807:U:OP2 | 34:YP:41:ARG:NH1 | 2.40 | 0.55 |
| 1:XA:1151:A:H2' | 1:XA:1152:A:C8 | 2.42 | 0.55 |
| 1:XA:587:G:H22 | 1:XA:754:C:P | 2.30 | 0.55 |
| 1:QA:45:U:H2' | 1:QA:46:G:C8 | 2.42 | 0.55 |
| 1:QA:742:G:OP2 | 15:QO:35:ARG:NH2 | 2.39 | 0.55 |
| 1:QA:985:C:H2' | 1:QA:986:A:H8 | 1.70 | 0.55 |
| 3:QC:5:ILE:HD13 | 10:QJ:51:ARG:HH21 | 1.72 | 0.55 |
| 1:XA:410:G:H4' | 1:XA:411:A:OP1 | 2.06 | 0.55 |
| 1:QA:1372:U:H5'' | 9:QI:71:SER:HB3 | 1.89 | 0.54 |
| 1:QA:1414:U:H2' | 1:QA:1415:G:H8 | 1.73 | 0.54 |
| 2:QB:84:GLU:HB3 | 2:QB:219:VAL:HG21 | 1.88 | 0.54 |
| 1:QA:545:C:H5' | 4:QD:72:GLU:HG3 | 1.89 | 0.54 |
| 24:RA:10:G:O2' | 24:RA:2801:A:O2' | 2.25 | 0.54 |
| 24:RA:2696:U:H2' | 24:RA:2697:G:H8 | 1.72 | 0.54 |
| 24:RA:517:C:HO2' | 41:RW:18:ARG:HH22 | 1.52 | 0.54 |
| 3:XC:88:ARG:HA | 3:XC:91:LEU:HD12 | 1.90 | 0.54 |
| 26:YD:50:THR:OG1 | 26:YD:51:VAL:N | 2.40 | 0.54 |
| 24:RA:620:G:H4' | 24:RA:621:A:H5'' | 1.89 | 0.54 |
| 29:RG:63:ILE:HG22 | 29:RG:143:GLU:HB2 | 1.88 | 0.54 |
| 1:XA:902:G:H2' | 1:XA:903:G:H8 | 1.73 | 0.54 |
| 11:XK:33:THR:HA | 11:XK:39:PRO:HA | 1.89 | 0.54 |
| 24:YA:1316:U:H2' | 24:YA:1317:A:C8 | 2.42 | 0.54 |
| 24:YA:676:A:H8 | 24:YA:2069:G:H21 | 1.53 | 0.54 |
| 24:YA:994:C:OP2 | 39:YU:54:LYS:NZ | 2.33 | 0.54 |
| 38:YT:50:ILE:HD11 | 38:YT:100:TYR:HA | 1.89 | 0.54 |
| 43:YY:102:CYS:SG | 43:YY:103:GLY:N | 2.80 | 0.54 |
| 24:RA:1026:U:H4' | 24:RA:1027:A:OP1 | 2.07 | 0.54 |
| 24:RA:1824:G:N3 | 26:RD:254:THR:OG1 | 2.40 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:RA:74:A:H4' | 24:RA:75:G:O5' | 2.07 | 0.54 |
| 4:XD:61:LYS:CG | 4:XD:61:LYS:NZ | 2.69 | 0.54 |
| 24:YA:1645:G:H5'' | 24:YA:1646:C:H5' | 1.88 | 0.54 |
| 24:RA:2355:C:H4' | 45:R0:24:LYS:HG3 | 1.89 | 0.54 |
| 27:RE:48:GLN:OE1 | 27:RE:64:LYS:NZ | 2.37 | 0.54 |
| 38:RT:51:ARG:NH1 | 38:RT:100:TYR:OH | 2.40 | 0.54 |
| 44:RZ:102:LEU:HD11 | 44:RZ:124:ILE:HG12 | 1.90 | 0.54 |
| 1:XA:1304:G:H21 | 1:XA:1333:A:H62 | 1.54 | 0.54 |
| 13:XM:3:ARG:HA | 13:XM:9:ILE:HG21 | 1.89 | 0.54 |
| 24:YA:947:G:H2' | 24:YA:948:G:H8 | 1.72 | 0.54 |
| 32:YN:26:LEU:O | 32:YN:30:ILE:HG12 | 2.08 | 0.54 |
| 33:YO:87:ILE:HD12 | 33:YO:91:LEU:HA | 1.90 | 0.54 |
| 24:YA:958:U:OP2 | 35:YQ:14:ARG:NH1 | 2.41 | 0.54 |
| 1:QA:1504:G:H4' | 1:QA:1505:G:O5' | 2.08 | 0.54 |
| 50:R5:33:CYS:HB2 | 50:R5:40:LYS:HD3 | 1.87 | 0.54 |
| 24:RA:2304:G:H5' | 29:RG:124:SER:OG | 2.08 | 0.54 |
| 24:RA:2876:G:O2' | 38:RT:3:ARG:NH1 | 2.40 | 0.54 |
| 24:RA:589:C:H2' | 24:RA:590:A:C8 | 2.43 | 0.54 |
| 26:RD:147:LEU:HD23 | 26:RD:148:GLU:HG3 | 1.89 | 0.54 |
| 24:RA:566:U:H5'' | 34:RP:29:LYS:HE3 | 1.90 | 0.54 |
| 2:XB:47:THR:HG23 | 2:XB:202:PRO:HG2 | 1.89 | 0.54 |
| 4:XD:145:GLU:HG3 | 4:XD:184:LYS:HE2 | 1.88 | 0.54 |
| 1:XA:405:U:O4 | 4:XD:2:GLY:N | 2.41 | 0.54 |
| 7:XG:23:VAL:O | 7:XG:27:ILE:HG12 | 2.08 | 0.54 |
| 24:YA:1062:G:H2' | 24:YA:1063:G:C8 | 2.42 | 0.54 |
| 24:YA:1830:C:H2' | 24:YA:1831:G:H8 | 1.72 | 0.54 |
| 35:YQ:81:VAL:O | 35:YQ:82:ARG:NE | 2.29 | 0.54 |
| 43:YY:1:MET:HG3 | 43:YY:2:ARG:H | 1.72 | 0.54 |
| 1:QA:1287:A:H2' | 1:QA:1288:A:C8 | 2.43 | 0.54 |
| 1:QA:486:U:H2' | 1:QA:487:A:H8 | 1.72 | 0.54 |
| 24:RA:2420:C:H5' | 51:R6:54:ILE:HD11 | 1.90 | 0.54 |
| 24:RA:270(N):G:OP1 | 31:RI:57:ARG:NH1 | 2.36 | 0.54 |
| 24:RA:2749:A:OP1 | 30:RH:4:ILE:HG23 | 2.08 | 0.54 |
| 34:RP:126:VAL:HG13 | 34:RP:147:LEU:HD21 | 1.89 | 0.54 |
| 4:XD:64:LEU:HA | 4:XD:67:ILE:HD12 | 1.89 | 0.54 |
| 9:XI:10:ARG:HD2 | 9:XI:105:ASP:HB2 | 1.89 | 0.54 |
| 24:YA:270(E):G:H1 | 24:YA:270(U):C:H42 | 1.54 | 0.54 |
| 39:YU:29:SER:OG | 39:YU:30:LYS:NZ | 2.34 | 0.54 |
| 1:QA:1060:C:H2' | 1:QA:1061:G:H8 | 1.72 | 0.54 |
| 1:QA:1346:A:H5'' | 9:QI:120:ARG:HH12 | 1.73 | 0.54 |
| 24:RA:2133:G:H1' | 24:RA:2158:A:H61 | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:RP:47:ASP:OD2 | 53:R8:59:LYS:NZ | 2.41 | 0.54 |
| 44:RZ:145:GLU:HG3 | 44:RZ:146:ILE:HG12 | 1.89 | 0.54 |
| 1:XA:1085:U:OP1 | 1:XA:1094:G:N2 | 2.41 | 0.54 |
| 1:XA:1287:A:H2' | 1:XA:1288:A:C8 | 2.43 | 0.54 |
| 5:XE:33:VAL:HG23 | 5:XE:112:LEU:HD22 | 1.89 | 0.54 |
| 8:XH:21:LYS:HD3 | 8:XH:24:THR:HG22 | 1.90 | 0.54 |
| 24:YA:1338:G:N7 | 42:YX:62:LYS:NZ | 2.49 | 0.54 |
| 24:YA:2795:G:N2 | 24:YA:2799:A:OP2 | 2.41 | 0.54 |
| 1:QA:1451:A:H5'' | 1:QA:1452:C:H5' | 1.89 | 0.54 |
| 4:QD:12:CYS:HB3 | 4:QD:33:MET:HE2 | 1.89 | 0.54 |
| 13:QM:17:VAL:HA | 13:QM:20:THR:HG23 | 1.90 | 0.54 |
| 20:QT:85:MET:HA | 20:QT:88:VAL:HG22 | 1.89 | 0.54 |
| 24:RA:2022:U:OP2 | 50:R5:15:ARG:NH2 | 2.41 | 0.54 |
| 24:RA:1341:U:OP1 | 24:RA:1397:U:N3 | 2.36 | 0.54 |
| 24:RA:2137:C:H42 | 24:RA:2154:G:H1 | 1.56 | 0.54 |
| 24:RA:270(S):G:H2' | 24:RA:270(T):G:H8 | 1.72 | 0.54 |
| 24:RA:466:A:OP1 | 52:R7:34:ARG:NH1 | 2.40 | 0.54 |
| 24:RA:605:C:O2 | 24:RA:657:U:O2' | 2.26 | 0.54 |
| 24:RA:675:A:N3 | 24:RA:2443:C:O2' | 2.37 | 0.54 |
| 24:RA:1818:U:H2' | 26:RD:157:ARG:HG2 | 1.90 | 0.54 |
| 30:RH:101:ARG:HE | 30:RH:117:PRO:HG2 | 1.73 | 0.54 |
| 1:XA:718:G:O6 | 18:XR:74:ARG:NH1 | 2.40 | 0.54 |
| 24:YA:1022:G:O2' | 24:YA:1023:U:OP2 | 2.22 | 0.54 |
| 24:YA:1105:U:H2' | 24:YA:1106:G:H8 | 1.72 | 0.54 |
| 24:YA:1231:G:H2' | 24:YA:1232:G:H8 | 1.73 | 0.54 |
| 24:YA:1859:A:N6 | 24:YA:1883:G:HO2' | 2.06 | 0.54 |
| 24:YA:2882:A:OP1 | 36:YR:96:ARG:NH1 | 2.36 | 0.54 |
| 1:QA:165:C:H2' | 1:QA:166:G:H8 | 1.73 | 0.54 |
| 1:QA:410:G:H4' | 1:QA:411:A:OP1 | 2.07 | 0.54 |
| 1:QA:736:C:H2' | 1:QA:737:A:C8 | 2.43 | 0.54 |
| 1:QA:833:U:H3 | 1:QA:853:G:H1 | 1.56 | 0.54 |
| 1:QA:831:U:H3 | 1:QA:855:G:H1 | 1.56 | 0.54 |
| 14:QN:21:TYR:OH | 14:QN:23:ARG:NH2 | 2.39 | 0.54 |
| 18:QR:74:ARG:HD3 | 18:QR:81:PHE:HA | 1.90 | 0.54 |
| 24:RA:2539:C:H5' | 54:R9:3:VAL:HG21 | 1.89 | 0.54 |
| 24:RA:1085:A:H2' | 24:RA:1086:A:C4 | 2.43 | 0.54 |
| 5:XE:37:ARG:NH1 | 5:XE:111:GLU:O | 2.41 | 0.54 |
| 24:YA:1062:G:H22 | 24:YA:1078:U:H1' | 1.72 | 0.54 |
| 24:YA:2469:A:H2 | 24:YA:2481:G:H21 | 1.56 | 0.54 |
| 24:YA:581:C:H2' | 24:YA:582:G:C8 | 2.43 | 0.54 |
| 1:QA:1412:C:H2' | 1:QA:1413:A:C8 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:QA:1510:U:H2' | 1:QA:1511:G:C8 | 2.42 | 0.54 |
| 1:QA:501:C:H1' | 1:QA:549:C:H1' | 1.90 | 0.54 |
| 24:RA:184:C:O2' | 24:RA:217:G:N3 | 2.41 | 0.54 |
| 32:RN:133:GLN:HG3 | 32:RN:135:PRO:HD3 | 1.89 | 0.54 |
| 44:RZ:7:ALA:HB2 | 44:RZ:59:LEU:HB3 | 1.90 | 0.54 |
| 1:XA:436:C:H1' | 4:XD:157:LEU:HD22 | 1.89 | 0.54 |
| 1:XA:581:G:OP1 | 15:XO:65:ARG:NH1 | 2.37 | 0.54 |
| 24:YA:1537:C:H2' | 24:YA:1538:G:C8 | 2.42 | 0.54 |
| 24:YA:964:C:O2' | 24:YA:2273:A:N3 | 2.36 | 0.54 |
| 24:YA:309:G:N3 | 24:YA:329:G:O2' | 2.41 | 0.54 |
| 6:QF:99:ALA:HB1 | 18:QR:23:LYS:HE3 | 1.90 | 0.53 |
| 1:QA:642:A:N3 | 8:QH:113:SER:OG | 2.40 | 0.53 |
| 24:RA:579:G:O2' | 24:RA:2019:A:OP1 | 2.22 | 0.53 |
| 24:RA:459:U:H2' | 24:RA:460:A:H8 | 1.73 | 0.53 |
| 27:RE:50:GLY:HA2 | 27:RE:77:ILE:HA | 1.90 | 0.53 |
| 1:XA:410:G:N2 | 1:XA:432:A:H62 | 2.05 | 0.53 |
| 24:YA:2233:U:H2' | 24:YA:2234:G:C8 | 2.43 | 0.53 |
| 35:YQ:66:ILE:HA | 35:YQ:104:PHE:HA | 1.90 | 0.53 |
| 1:QA:1342:C:H2' | 1:QA:1343:G:C8 | 2.44 | 0.53 |
| 11:QK:22:HIS:HB3 | 11:QK:29:ILE:HG13 | 1.90 | 0.53 |
| 13:QM:23:TYR:HE2 | 13:QM:70:LEU:HB2 | 1.72 | 0.53 |
| 22:QV:20:G:H5' | 22:QV:21:U:H5 | 1.73 | 0.53 |
| 50:R5:41:PRO:O | 50:R5:44:THR:OG1 | 2.25 | 0.53 |
| 24:RA:1035:U:H2' | 24:RA:1036:G:C8 | 2.43 | 0.53 |
| 24:RA:1972:A:H2' | 24:RA:1973:G:H8 | 1.72 | 0.53 |
| 24:RA:307:G:H3' | 24:RA:307:G:C8 | 2.43 | 0.53 |
| 24:RA:848:G:H2' | 24:RA:849:A:C8 | 2.43 | 0.53 |
| 24:RA:861:A:N3 | 25:RB:79:C:O2' | 2.40 | 0.53 |
| 37:RS:27:SER:HB3 | 37:RS:38:GLN:HB3 | 1.88 | 0.53 |
| 24:RA:138:G:N2 | 42:RX:44:GLU:OE1 | 2.37 | 0.53 |
| 1:XA:1342:C:H2' | 1:XA:1343:G:C8 | 2.44 | 0.53 |
| 1:XA:79:G:H1 | 1:XA:90:C:H42 | 1.56 | 0.53 |
| 4:XD:139:ARG:NH1 | 4:XD:140:VAL:O | 2.41 | 0.53 |
| 1:XA:376:G:H5'' | 16:XP:5:ARG:HB2 | 1.90 | 0.53 |
| 24:YA:1996:C:OP1 | 33:YO:31:LYS:NZ | 2.41 | 0.53 |
| 24:YA:1006:C:H5' | 32:YN:28:THR:HG23 | 1.91 | 0.53 |
| 44:YZ:72:ARG:NH2 | 44:YZ:97:GLU:O | 2.30 | 0.53 |
| 1:QA:1010:G:H2' | 1:QA:1011:G:H8 | 1.72 | 0.53 |
| 1:QA:21:G:H2' | 1:QA:22:G:C8 | 2.43 | 0.53 |
| 1:QA:368:U:OP1 | 31:YI:91:SER:OG | 2.23 | 0.53 |
| 44:RZ:128:VAL:HG12 | 44:RZ:129:SER:H | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:XA:356:A:N3 | 1:XA:368:U:O2' | 2.32 | 0.53 |
| 19:XS:63:THR:H | 19:XS:66:MET:HE3 | 1.74 | 0.53 |
| 24:YA:631:A:OP2 | 53:Y8:46:ARG:NH2 | 2.41 | 0.53 |
| 1:QA:137:C:H2' | 1:QA:138:G:H8 | 1.72 | 0.53 |
| 1:QA:410:G:H21 | 1:QA:432:A:H62 | 1.54 | 0.53 |
| 24:RA:1012:U:OP1 | 39:RU:75:ASN:ND2 | 2.38 | 0.53 |
| 24:RA:1315:C:O2' | 24:RA:1392:A:N3 | 2.35 | 0.53 |
| 24:RA:1542:G:O6 | 24:RA:1543:A:N6 | 2.42 | 0.53 |
| 24:RA:177:G:H5' | 24:RA:178:G:C8 | 2.43 | 0.53 |
| 24:RA:2031:A:N3 | 24:RA:2455:G:O2' | 2.37 | 0.53 |
| 24:RA:262:A:N3 | 24:RA:430:G:O2' | 2.33 | 0.53 |
| 24:RA:822:U:H2' | 24:RA:823:G:H8 | 1.72 | 0.53 |
| 38:RT:24:PRO:HG3 | 38:RT:52:ILE:HG22 | 1.90 | 0.53 |
| 1:XA:34:C:H2' | 1:XA:35:G:C8 | 2.44 | 0.53 |
| 1:XA:711:G:H2' | 1:XA:712:A:H8 | 1.74 | 0.53 |
| 9:XI:63:ILE:HG21 | 9:XI:77:ILE:HD12 | 1.91 | 0.53 |
| 24:YA:2070:G:H2' | 24:YA:2071:A:C8 | 2.44 | 0.53 |
| 24:YA:2638:G:OP1 | 27:YE:82:ARG:NH2 | 2.42 | 0.53 |
| 24:YA:2683:C:OP1 | 38:YT:53:ARG:NH2 | 2.33 | 0.53 |
| 27:YE:36:ARG:NH1 | 27:YE:85:ASN:OD1 | 2.40 | 0.53 |
| 3:QC:19:GLU:O | 3:QC:40:ARG:NH2 | 2.41 | 0.53 |
| 10:QJ:78:ASN:O | 10:QJ:81:THR:OG1 | 2.25 | 0.53 |
| 47:R2:4:SER:OG | 47:R2:5:GLU:N | 2.41 | 0.53 |
| 26:RD:72:LYS:HD2 | 26:RD:75:ILE:HD12 | 1.90 | 0.53 |
| 1:XA:324:G:P | 20:XT:22:ARG:HE | 2.31 | 0.53 |
| 1:XA:452:A:N6 | 1:XA:480:U:H3 | 1.97 | 0.53 |
| 5:XE:103:GLY:O | 5:XE:106:PRO:HD2 | 2.08 | 0.53 |
| 8:XH:29:SER:HB3 | 8:XH:32:LYS:HD2 | 1.90 | 0.53 |
| 24:YA:1124:C:O2 | 54:Y9:36:GLN:NE2 | 2.41 | 0.53 |
| 1:QA:509:A:H4' | 1:QA:510:A:OP1 | 2.07 | 0.53 |
| 50:R5:56:LYS:NZ | 50:R5:59:GLU:OE1 | 2.41 | 0.53 |
| 24:RA:2329:G:H2' | 24:RA:2330:G:C8 | 2.44 | 0.53 |
| 24:RA:783:A:H8 | 24:RA:784:A:H4' | 1.73 | 0.53 |
| 33:RO:15:GLY:HA2 | 33:RO:47:ILE:HG12 | 1.90 | 0.53 |
| 1:XA:624:C:H2' | 1:XA:625:G:H8 | 1.72 | 0.53 |
| 24:YA:300:A:OP1 | 43:YY:86:ARG:NH2 | 2.41 | 0.53 |
| 24:YA:947:G:H2' | 24:YA:948:G:C8 | 2.44 | 0.53 |
| 29:YG:161:THR:HG22 | 29:YG:163:ALA:H | 1.74 | 0.53 |
| 1:QA:982:U:O2 | 1:QA:1222:G:N1 | 2.40 | 0.53 |
| 1:QA:324:G:N1 | 1:QA:327:A:OP2 | 2.41 | 0.53 |
| 1:QA:300:A:O2' | 1:QA:564:C:N3 | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:689:C:OP2 | 11:QK:55:LYS:NZ | 2.38 | 0.53 |
| 11:QK:34:ASP:OD1 | 11:QK:38:ASN:N | 2.42 | 0.53 |
| 24:RA:2081:C:H2' | 24:RA:2082:A:H8 | 1.73 | 0.53 |
| 24:RA:2859:G:H2' | 24:RA:2860:A:C8 | 2.44 | 0.53 |
| 24:RA:1657:C:C3' | 27:RE:133:LYS:HG2 | 2.38 | 0.53 |
| 1:XA:266:G:O2' | 1:XA:267:C:OP2 | 2.23 | 0.53 |
| 1:XA:359:U:O5' | 1:XA:359:U:C6 | 2.62 | 0.53 |
| 1:XA:692:U:OP1 | 11:XK:124:LYS:NZ | 2.31 | 0.53 |
| 24:YA:2528:U:O2' | 24:YA:2530:A:OP1 | 2.21 | 0.53 |
| 24:YA:521:G:H2' | 24:YA:522:G:H8 | 1.74 | 0.53 |
| 37:YS:14:VAL:O | 37:YS:18:ILE:HG12 | 2.09 | 0.53 |
| 24:YA:1155:A:O3' | 39:YU:55:ARG:NH1 | 2.41 | 0.53 |
| 1:QA:1227:A:N3 | 19:QS:83:HIS:ND1 | 2.57 | 0.53 |
| 1:QA:45:U:H2' | 1:QA:46:G:H8 | 1.73 | 0.53 |
| 24:RA:1230:C:H2' | 24:RA:1231:G:H8 | 1.74 | 0.53 |
| 24:RA:1360:A:H62 | 24:RA:1371:G:H21 | 1.57 | 0.53 |
| 24:RA:1266:G:O2' | 24:RA:2012:G:O6 | 2.22 | 0.53 |
| 24:RA:919:G:N2 | 24:RA:2269:A:OP2 | 2.41 | 0.53 |
| 24:RA:512:G:H4' | 24:RA:513:A:O5' | 2.09 | 0.53 |
| 26:RD:136:ILE:O | 26:RD:168:ARG:NH2 | 2.41 | 0.53 |
| 1:XA:1129:C:N4 | 1:XA:1135:U:O4 | 2.42 | 0.53 |
| 1:XA:189:U:O2 | 17:XQ:63:ARG:NH2 | 2.42 | 0.53 |
| 18:XR:67:ALA:HA | 18:XR:70:ILE:HD12 | 1.91 | 0.53 |
| 24:YA:743:G:O2' | 24:YA:1659:U:OP1 | 2.22 | 0.53 |
| 1:QA:345:C:H3' | 38:RT:41:ARG:HH12 | 1.72 | 0.53 |
| 1:QA:99:C:H2' | 1:QA:101:A:C8 | 2.42 | 0.53 |
| 24:RA:1061:U:H5'' | 24:RA:1070:A:H1' | 1.90 | 0.53 |
| 24:RA:1485:G:H1 | 24:RA:1504:C:H42 | 1.57 | 0.53 |
| 24:RA:391:G:O2' | 24:RA:410:G:OP1 | 2.25 | 0.53 |
| 24:RA:679:C:H2' | 24:RA:680:G:H8 | 1.73 | 0.53 |
| 28:RF:124:LEU:HD12 | 28:RF:191:ARG:HH21 | 1.73 | 0.53 |
| 29:RG:161:THR:HG22 | 29:RG:163:ALA:H | 1.74 | 0.53 |
| 1:XA:64:G:H5'' | 1:XA:65:U:OP1 | 2.09 | 0.53 |
| 24:YA:1062:G:H2' | 24:YA:1063:G:H8 | 1.74 | 0.53 |
| 24:YA:1802:A:H2' | 24:YA:1803:A:C8 | 2.43 | 0.53 |
| 24:YA:2030:A:H4' | 24:YA:2031:A:C8 | 2.44 | 0.53 |
| 24:YA:387:U:OP1 | 46:Y1:20:ARG:NH1 | 2.35 | 0.53 |
| 24:YA:603:A:N1 | 24:YA:625:G:O2' | 2.35 | 0.53 |
| 24:YA:840:C:H2' | 24:YA:841:A:C8 | 2.44 | 0.53 |
| 27:YE:18:ASP:HB3 | 38:YT:82:LEU:HD21 | 1.91 | 0.53 |
| 1:QA:1064:G:H1' | 1:QA:1066:C:C6 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:QA:1252:A:H61 | 1:QA:1285:A:H61 | 1.55 | 0.53 |
| 24:RA:1403:C:H5'' | 24:RA:1471:A:H1' | 1.91 | 0.53 |
| 24:RA:2006:C:O2' | 24:RA:2823:A:N3 | 2.41 | 0.53 |
| 24:RA:2352:A:N6 | 24:RA:2365:G:O2' | 2.42 | 0.53 |
| 24:RA:2515:C:H2' | 24:RA:2516:G:H8 | 1.74 | 0.53 |
| 34:RP:100:LEU:HB2 | 34:RP:106:LEU:HG | 1.90 | 0.53 |
| 1:XA:407:G:H2' | 1:XA:408:A:H8 | 1.73 | 0.53 |
| 1:XA:688:G:O2' | 1:XA:704:A:N1 | 2.35 | 0.53 |
| 3:XC:121:ALA:O | 3:XC:125:GLU:HG3 | 2.09 | 0.53 |
| 7:XG:116:ALA:HA | 7:XG:119:ARG:HE | 1.74 | 0.53 |
| 9:XI:13:ALA:HB2 | 9:XI:68:GLY:HA3 | 1.91 | 0.53 |
| 1:XA:263:A:OP2 | 20:XT:79:ARG:NH1 | 2.42 | 0.53 |
| 1:XA:1235:U:H5'' | 21:XU:3:LYS:HD2 | 1.90 | 0.53 |
| 24:YA:252:G:OP2 | 34:YP:50:ARG:NH1 | 2.41 | 0.53 |
| 24:YA:442:G:H1' | 28:YF:48:THR:HG21 | 1.91 | 0.53 |
| 1:QA:1479:C:H2' | 1:QA:1480:G:H8 | 1.74 | 0.52 |
| 1:QA:152:A:H62 | 1:QA:169:C:H42 | 1.57 | 0.52 |
| 1:QA:152:A:H62 | 1:QA:169:C:N4 | 2.07 | 0.52 |
| 1:QA:181:G:O2' | 1:QA:182:U:O5' | 2.27 | 0.52 |
| 1:QA:352:C:O2' | 1:QA:354:G:OP1 | 2.20 | 0.52 |
| 24:RA:2729:G:H1' | 27:RE:187:ALA:HB2 | 1.89 | 0.52 |
| 24:RA:380:U:H2' | 24:RA:381:G:H8 | 1.73 | 0.52 |
| 29:RG:71:THR:N | 29:RG:89:GLY:O | 2.41 | 0.52 |
| 1:XA:770:C:H2' | 1:XA:771:G:H8 | 1.74 | 0.52 |
| 8:XH:32:LYS:HA | 8:XH:35:ILE:HD12 | 1.90 | 0.52 |
| 10:XJ:62:HIS:HD1 | 14:XN:59:ALA:HB3 | 1.74 | 0.52 |
| 24:YA:439:G:H2' | 24:YA:440:G:H8 | 1.75 | 0.52 |
| 24:YA:881:G:H3' | 24:YA:882:G:C8 | 2.44 | 0.52 |
| 24:YA:949:C:H2' | 24:YA:950:G:H8 | 1.74 | 0.52 |
| 40:YV:60:GLU:OE1 | 40:YV:97:LYS:NZ | 2.42 | 0.52 |
| 3:QC:78:GLY:HA3 | 3:QC:83:ARG:HB2 | 1.92 | 0.52 |
| 24:RA:1152:C:H2' | 24:RA:1153:C:C6 | 2.44 | 0.52 |
| 24:RA:1358:G:N1 | 24:RA:1372:U:OP2 | 2.35 | 0.52 |
| 24:RA:589:C:H2' | 24:RA:590:A:H8 | 1.72 | 0.52 |
| 24:RA:859:G:N2 | 24:RA:917:A:OP2 | 2.35 | 0.52 |
| 35:RQ:27:VAL:HG11 | 35:RQ:134:ARG:HA | 1.90 | 0.52 |
| 39:RU:58:ARG:O | 39:RU:62:ILE:HG12 | 2.09 | 0.52 |
| 44:RZ:123:ASP:N | 44:RZ:123:ASP:OD1 | 2.42 | 0.52 |
| 24:YA:2011:U:OP2 | 41:YW:16:LYS:NZ | 2.36 | 0.52 |
| 43:YY:39:VAL:HG13 | 43:YY:42:VAL:HB | 1.90 | 0.52 |
| 34:RP:49:ARG:HH11 | 53:R8:58:ILE:HG22 | 1.73 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:RA:1405:U:H2' | 24:RA:1406:U:H6 | 1.75 | 0.52 |
| 24:RA:2630:G:H2' | 24:RA:2631:G:H8 | 1.73 | 0.52 |
| 30:RH:164:TYR:HB2 | 30:RH:167:GLU:HB2 | 1.90 | 0.52 |
| 38:RT:5:ALA:HA | 38:RT:8:LYS:HD3 | 1.91 | 0.52 |
| 1:XA:1446:A:HO2' | 1:XA:1447:G:P | 2.32 | 0.52 |
| 14:YN:24:CYS:HB2 | 14:YN:29:ARG:H | 1.75 | 0.52 |
| 24:YA:140:A:H8 | 24:YA:1408:C:HO2' | 1.56 | 0.52 |
| 24:YA:2345:G:H5' | 24:YA:2347:C:O4' | 2.10 | 0.52 |
| 24:YA:436:C:H2' | 24:YA:438:G:H8 | 1.74 | 0.52 |
| 24:YA:956:G:N2 | 24:YA:960:A:OP2 | 2.42 | 0.52 |
| 1:QA:817:C:O2' | 1:QA:1527:C:H5' | 2.08 | 0.52 |
| 1:QA:22:G:H2' | 1:QA:23:C:C6 | 2.45 | 0.52 |
| 1:QA:624:C:H2' | 1:QA:625:G:H8 | 1.74 | 0.52 |
| 9:QI:24:GLY:N | 9:QI:60:ASP:OD1 | 2.40 | 0.52 |
| 24:RA:1479:G:OP2 | 24:RA:1510:A:N6 | 2.41 | 0.52 |
| 24:RA:2037:G:H2' | 24:RA:2038:G:C8 | 2.45 | 0.52 |
| 24:RA:964:C:O2' | 24:RA:2273:A:N3 | 2.39 | 0.52 |
| 24:RA:2392:A:OP2 | 24:RA:2422:A:N6 | 2.42 | 0.52 |
| 37:RS:14:VAL:O | 37:RS:18:ILE:HG12 | 2.09 | 0.52 |
| 41:RW:92:ARG:HH21 | 41:RW:94:ASP:HA | 1.73 | 0.52 |
| 1:XA:224:C:H2' | 1:XA:225:C:C6 | 2.44 | 0.52 |
| 4:XD:127:THR:HA | 4:XD:132:ARG:HA | 1.92 | 0.52 |
| 4:XD:61:LYS:NZ | 4:XD:72:GLU:OE2 | 2.22 | 0.52 |
| 24:YA:1506:C:H2' | 24:YA:1507:A:H5'' | 1.90 | 0.52 |
| 24:YA:1593:G:H2' | 24:YA:1594:G:C8 | 2.45 | 0.52 |
| 24:YA:2032:G:OP2 | 24:YA:2454:G:O2' | 2.26 | 0.52 |
| 24:YA:2700:C:O2' | 24:YA:2701:C:H5' | 2.09 | 0.52 |
| 24:YA:414:C:H2' | 24:YA:415:A:C8 | 2.44 | 0.52 |
| 24:YA:863:A:H2' | 24:YA:864:G:H8 | 1.74 | 0.52 |
| 30:YH:164:TYR:HB2 | 30:YH:167:GLU:HB2 | 1.91 | 0.52 |
| 44:YZ:166:SER:HB3 | 44:YZ:168:GLU:N | 2.25 | 0.52 |
| 44:YZ:4:ARG:HH11 | 44:YZ:60:GLU:HG2 | 1.75 | 0.52 |
| 1:QA:946:A:O2' | 1:QA:1333:A:N3 | 2.39 | 0.52 |
| 2:QB:47:THR:O | 2:QB:51:LEU:HG | 2.09 | 0.52 |
| 5:QE:81:GLU:HG2 | 5:QE:90:VAL:HG23 | 1.90 | 0.52 |
| 24:RA:2683:C:OP1 | 38:RT:53:ARG:NH2 | 2.36 | 0.52 |
| 36:RR:56:LYS:NZ | 36:RR:90:ARG:O | 2.43 | 0.52 |
| 20:XT:83:ARG:O | 20:XT:87:LYS:HG3 | 2.10 | 0.52 |
| 24:YA:2181:G:H2' | 24:YA:2182:G:C8 | 2.44 | 0.52 |
| 26:YD:168:ARG:HG2 | 26:YD:173:VAL:HG12 | 1.91 | 0.52 |
| 30:YH:4:ILE:HB | 30:YH:6:ARG:HH11 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 34:YP:135:LEU:HG | 34:YP:139:LYS:HE2 | 1.92 | 0.52 |
| 35:YQ:75:THR:HG21 | 35:YQ:85:LYS:HE3 | 1.91 | 0.52 |
| 1:QA:1129:C:H5' | 1:QA:1130:A:H5' | 1.92 | 0.52 |
| 1:QA:1386:G:H2' | 1:QA:1387:G:H8 | 1.75 | 0.52 |
| 1:QA:28:G:O2' | 1:QA:296:U:OP1 | 2.26 | 0.52 |
| 4:QD:74:GLN:O | 4:QD:78:LEU:HG | 2.10 | 0.52 |
| 25:RB:52:A:H2 | 25:RB:53:A:H62 | 1.57 | 0.52 |
| 27:RE:45:THR:O | 27:RE:83:ASP:N | 2.41 | 0.52 |
| 1:XA:45:U:H2' | 1:XA:46:G:C8 | 2.44 | 0.52 |
| 1:XA:573:A:N3 | 1:XA:883:C:O2' | 2.38 | 0.52 |
| 1:XA:701:C:O2 | 1:XA:703:G:N1 | 2.43 | 0.52 |
| 8:XH:7:ALA:HB2 | 8:XH:85:ARG:HD3 | 1.90 | 0.52 |
| 13:XM:65:LYS:HD3 | 13:XM:69:GLU:HG3 | 1.92 | 0.52 |
| 24:YA:1422:G:H1 | 24:YA:1576:U:H3 | 1.58 | 0.52 |
| 24:YA:1636:C:H2' | 24:YA:1637:A:C8 | 2.44 | 0.52 |
| 1:QA:1002:G:H2' | 1:QA:1003:G:H8 | 1.75 | 0.52 |
| 1:QA:1159:U:O2' | 1:QA:1160:G:N7 | 2.40 | 0.52 |
| 1:QA:119:A:H4' | 1:QA:120:A:O5' | 2.09 | 0.52 |
| 1:QA:986:A:N3 | 19:QS:52:TYR:OH | 2.35 | 0.52 |
| 1:QA:1071:C:H5'' | 5:QE:49:PRO:HG2 | 1.92 | 0.52 |
| 7:QG:24:THR:HA | 7:QG:27:ILE:HG12 | 1.91 | 0.52 |
| 8:QH:19:VAL:HG13 | 8:QH:21:LYS:HG3 | 1.91 | 0.52 |
| 9:QI:104:ARG:NH1 | 9:QI:105:ASP:O | 2.43 | 0.52 |
| 47:R2:45:SER:O | 47:R2:46:GLN:NE2 | 2.43 | 0.52 |
| 1:XA:1071:C:H2' | 1:XA:1072:G:H8 | 1.75 | 0.52 |
| 1:XA:1172:C:H2' | 1:XA:1173:G:H8 | 1.74 | 0.52 |
| 1:XA:1408:A:C6 | 1:XA:1494:G:C6 | 2.98 | 0.52 |
| 49:Y4:62:ARG:HD3 | 49:Y4:63:TYR:H | 1.75 | 0.52 |
| 24:YA:2291:U:H2' | 24:YA:2292:C:C6 | 2.45 | 0.52 |
| 26:YD:25:THR:OG1 | 26:YD:26:LYS:N | 2.42 | 0.52 |
| 30:YH:153:LYS:HB3 | 30:YH:161:GLY:HA2 | 1.92 | 0.52 |
| 30:YH:8:PRO:HG2 | 30:YH:69:ARG:HE | 1.74 | 0.52 |
| 44:YZ:163:LEU:HD22 | 44:YZ:167:PRO:HG3 | 1.92 | 0.52 |
| 1:QA:1036:G:N7 | 1:QA:1037:C:N4 | 2.58 | 0.52 |
| 1:QA:825:G:O2' | 8:QH:12:ARG:NH2 | 2.40 | 0.52 |
| 2:QB:219:VAL:HA | 2:QB:222:ILE:HD12 | 1.92 | 0.52 |
| 20:QT:21:LYS:O | 20:QT:25:ARG:HG3 | 2.10 | 0.52 |
| 24:RA:2329:G:H2' | 24:RA:2330:G:H8 | 1.74 | 0.52 |
| 24:RA:2626:C:H2' | 24:RA:2627:G:C8 | 2.45 | 0.52 |
| 24:RA:265:A:N6 | 24:RA:427:U:O2' | 2.43 | 0.52 |
| 29:RG:9:ARG:O | 29:RG:13:GLU:HG3 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:XJ:46:ARG:HA | 10:XJ:64:GLU:HA | 1.91 | 0.52 |
| 24:YA:2344:U:OP1 | 51:Y6:37:ARG:HD3 | 2.10 | 0.52 |
| 24:YA:2401:U:OP1 | 51:Y6:18:ARG:NH2 | 2.40 | 0.52 |
| 24:YA:2805:G:H2' | 24:YA:2807:G:C8 | 2.45 | 0.52 |
| 26:YD:27:THR:HG21 | 26:YD:81:ALA:HB1 | 1.91 | 0.52 |
| 1:QA:628:G:H2' | 1:QA:629:G:C8 | 2.45 | 0.52 |
| 11:QK:122:LYS:HD3 | 11:QK:124:LYS:H | 1.75 | 0.52 |
| 37:RS:20:ARG:NH1 | 45:R0:48:GLY:O | 2.43 | 0.52 |
| 24:RA:1035:U:O3' | 30:RH:59:ARG:NH1 | 2.42 | 0.52 |
| 24:RA:1354:A:H3' | 24:RA:1355:G:H8 | 1.75 | 0.52 |
| 24:RA:222:A:H62 | 24:RA:232:G:H21 | 1.57 | 0.52 |
| 24:RA:2443:C:H2' | 24:RA:2444:G:C8 | 2.45 | 0.52 |
| 24:RA:411:G:OP2 | 24:RA:2406:U:O2' | 2.17 | 0.52 |
| 24:RA:654(A):G:H1 | 24:RA:654(T):C:H42 | 1.56 | 0.52 |
| 1:XA:1288:A:O3' | 21:XU:10:ARG:NH1 | 2.43 | 0.52 |
| 1:XA:1299:A:C8 | 1:XA:1301:U:H1' | 2.45 | 0.52 |
| 1:XA:1414:U:H2' | 1:XA:1415:G:C8 | 2.45 | 0.52 |
| 1:XA:21:G:H2' | 1:XA:22:G:H8 | 1.75 | 0.52 |
| 9:XI:53:VAL:HA | 9:XI:95:LYS:HE3 | 1.92 | 0.52 |
| 24:YA:1491:G:H2' | 24:YA:1492:G:H8 | 1.73 | 0.52 |
| 24:YA:253:C:OP2 | 53:Y8:5:LYS:NZ | 2.32 | 0.52 |
| 1:QA:1119:C:H2' | 1:QA:1120:G:C8 | 2.45 | 0.52 |
| 1:QA:444:C:H2' | 1:QA:445:G:H8 | 1.75 | 0.52 |
| 2:QB:47:THR:HA | 2:QB:202:PRO:HG2 | 1.92 | 0.52 |
| 4:QD:163:GLU:HA | 4:QD:166:LYS:HE3 | 1.92 | 0.52 |
| 1:QA:954:G:O6 | 13:QM:104:ARG:NH1 | 2.42 | 0.52 |
| 24:RA:818:G:N1 | 24:RA:1188:U:OP2 | 2.27 | 0.52 |
| 24:RA:989:G:OP2 | 48:R3:11:SER:OG | 2.15 | 0.52 |
| 27:RE:12:THR:OG1 | 27:RE:13:ARG:N | 2.42 | 0.52 |
| 29:RG:41:GLN:HB3 | 29:RG:90:LEU:HB2 | 1.92 | 0.52 |
| 29:RG:67:LYS:HD2 | 49:R4:5:ILE:HD12 | 1.91 | 0.52 |
| 1:XA:1264:C:H2' | 1:XA:1265:G:C8 | 2.45 | 0.52 |
| 1:XA:243:A:H4' | 1:XA:244:U:H3' | 1.91 | 0.52 |
| 5:XE:35:GLY:HA3 | 5:XE:112:LEU:HB3 | 1.91 | 0.52 |
| 1:XA:452:A:O2' | 16:XP:72:ARG:NH1 | 2.43 | 0.52 |
| 24:YA:2228:G:OP1 | 26:YD:261:LYS:NZ | 2.28 | 0.52 |
| 24:YA:2632:A:HO2' | 24:YA:2811:G:HO2' | 1.58 | 0.52 |
| 24:YA:847:U:H5'' | 24:YA:847:U:H6 | 1.75 | 0.52 |
| 26:YD:13:ARG:HA | 26:YD:16:MET:HB2 | 1.92 | 0.52 |
| 32:YN:133:GLN:HG2 | 32:YN:135:PRO:HD3 | 1.92 | 0.52 |
| 33:YO:2:ILE:HB | 33:YO:33:ALA:HB3 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:985:C:H2' | 1:QA:986:A:C8 | 2.45 | 0.51 |
| 9:QI:63:ILE:HG21 | 9:QI:77:ILE:HD12 | 1.93 | 0.51 |
| 15:QO:87:ILE:HG22 | 15:QO:88:ARG:H | 1.76 | 0.51 |
| 17:QQ:21:VAL:HG11 | 17:QQ:59:ILE:HG13 | 1.91 | 0.51 |
| 24:RA:1316:U:H2' | 24:RA:1317:A:H8 | 1.75 | 0.51 |
| 24:RA:1399:C:H2' | 24:RA:1400:G:H8 | 1.75 | 0.51 |
| 24:RA:219:G:N3 | 24:RA:234:C:O2' | 2.42 | 0.51 |
| 24:RA:581:C:H2' | 24:RA:582:G:H8 | 1.74 | 0.51 |
| 26:RD:17:THR:O | 26:RD:211:ARG:NH1 | 2.40 | 0.51 |
| 30:RH:138:LYS:HA | 30:RH:141:VAL:HG22 | 1.91 | 0.51 |
| 1:XA:250:A:H4' | 1:XA:251:G:O5' | 2.09 | 0.51 |
| 1:XA:642:A:N3 | 8:XH:113:SER:OG | 2.41 | 0.51 |
| 10:XJ:77:PRO:HB2 | 10:XJ:79:ARG:HH22 | 1.74 | 0.51 |
| 1:XA:128:G:O2' | 17:XQ:3:LYS:NZ | 2.44 | 0.51 |
| 24:YA:1417:C:H2' | 24:YA:1418:G:O4' | 2.10 | 0.51 |
| 24:YA:2351:G:HO2' | 24:YA:2352:A:H8 | 1.59 | 0.51 |
| 24:YA:679:C:H2' | 24:YA:680:G:C8 | 2.44 | 0.51 |
| 25:YB:43:C:O3' | 29:YG:98:ARG:NH2 | 2.39 | 0.51 |
| 33:YO:24:VAL:HA | 33:YO:39:ILE:HG22 | 1.92 | 0.51 |
| 1:QA:946:A:H2' | 1:QA:947:G:H8 | 1.73 | 0.51 |
| 1:QA:599:C:O2' | 8:QH:129:VAL:O | 2.23 | 0.51 |
| 1:QA:1179:A:H5' | 9:QI:83:ARG:HH21 | 1.75 | 0.51 |
| 19:QS:51:VAL:O | 19:QS:57:HIS:HA | 2.10 | 0.51 |
| 24:RA:220:G:O2' | 24:RA:233:A:N3 | 2.42 | 0.51 |
| 26:RD:17:THR:HB | 26:RD:205:VAL:H | 1.74 | 0.51 |
| 29:RG:15:VAL:HG13 | 29:RG:175:LEU:HB2 | 1.91 | 0.51 |
| 36:RR:86:ARG:NH2 | 36:RR:118:GLU:OXT | 2.43 | 0.51 |
| 1:XA:1441:G:H21 | 1:XA:1460:A:N6 | 2.05 | 0.51 |
| 1:XA:377:G:H2' | 1:XA:378:G:H8 | 1.75 | 0.51 |
| 1:XA:529:G:O6 | 12:XL:49:ASN:ND2 | 2.43 | 0.51 |
| 1:XA:562:C:H1' | 12:XL:15:ARG:HD2 | 1.92 | 0.51 |
| 15:XO:39:LEU:HD23 | 15:XO:56:LEU:HB2 | 1.92 | 0.51 |
| 49:Y4:57:GLU:HG3 | 49:Y4:61:ARG:HG3 | 1.92 | 0.51 |
| 24:YA:1166:C:H2' | 24:YA:1167:U:C6 | 2.45 | 0.51 |
| 24:YA:2327:A:H2' | 24:YA:2328:A:C8 | 2.46 | 0.51 |
| 24:YA:2352:A:N6 | 24:YA:2365:G:O2' | 2.44 | 0.51 |
| 24:YA:675:A:OP1 | 28:YF:63:LYS:NZ | 2.35 | 0.51 |
| 24:YA:1005:C:O2' | 32:YN:28:THR:HG21 | 2.09 | 0.51 |
| 1:QA:1013:G:N2 | 1:QA:1016:A:OP2 | 2.36 | 0.51 |
| 1:QA:1065:U:O2' | 1:QA:1066:C:OP2 | 2.23 | 0.51 |
| 1:QA:663:A:H5'' | 18:QR:61:LYS:HE2 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 50:R5:16:ARG:NH1 | 50:R5:17:ASP:OD1 | 2.43 | 0.51 |
| 24:RA:1417:C:H2' | 24:RA:1418:G:O4' | 2.10 | 0.51 |
| 24:RA:2636:U:OP1 | 27:RE:80:GLU:N | 2.32 | 0.51 |
| 24:RA:2867:G:OP2 | 38:RT:119:LYS:NZ | 2.33 | 0.51 |
| 24:RA:309:G:OP2 | 24:RA:309:G:H8 | 1.93 | 0.51 |
| 24:RA:783:A:H2' | 24:RA:784:A:H4' | 1.91 | 0.51 |
| 35:RQ:66:ILE:HA | 35:RQ:104:PHE:HA | 1.91 | 0.51 |
| 40:RV:51:VAL:HG22 | 40:RV:53:GLU:H | 1.75 | 0.51 |
| 44:RZ:91:LEU:HD12 | 44:RZ:130:PRO:HB3 | 1.92 | 0.51 |
| 1:XA:1391:U:H2' | 1:XA:1392:G:C8 | 2.45 | 0.51 |
| 1:XA:1513:A:H2' | 1:XA:1514:C:C6 | 2.45 | 0.51 |
| 7:XG:20:ASP:HB3 | 7:XG:23:VAL:HG12 | 1.92 | 0.51 |
| 1:XA:35:G:H5' | 12:XL:104:VAL:CG2 | 2.41 | 0.51 |
| 24:YA:1224:G:OP2 | 40:YV:66:ARG:NH1 | 2.41 | 0.51 |
| 28:YF:65:TRP:NE1 | 28:YF:73:ALA:O | 2.37 | 0.51 |
| 29:YG:142:PRO:HB2 | 49:Y4:31:ILE:HG21 | 1.93 | 0.51 |
| 38:YT:3:ARG:HB2 | 38:YT:6:LEU:HB2 | 1.92 | 0.51 |
| 6:QF:30:LEU:HD23 | 6:QF:75:LEU:HD11 | 1.92 | 0.51 |
| 46:R1:83:GLU:HG2 | 46:R1:85:LEU:H | 1.73 | 0.51 |
| 24:RA:1131:G:HO2' | 24:RA:1132:A:H8 | 1.58 | 0.51 |
| 24:RA:1316:U:H2' | 24:RA:1317:A:C8 | 2.46 | 0.51 |
| 24:RA:2387:U:O2' | 45:R0:19:LYS:NZ | 2.44 | 0.51 |
| 29:RG:136:ARG:HH11 | 29:RG:137:GLU:HG2 | 1.76 | 0.51 |
| 40:RV:66:ARG:HH12 | 40:RV:88:ARG:HD3 | 1.75 | 0.51 |
| 1:XA:539:A:H2' | 1:XA:540:G:C8 | 2.46 | 0.51 |
| 2:XB:96:ARG:HH11 | 2:XB:98:LEU:HA | 1.75 | 0.51 |
| 24:YA:1510:A:O2' | 24:YA:1512:G:N7 | 2.40 | 0.51 |
| 24:YA:2102:U:H2' | 24:YA:2103:C:C6 | 2.46 | 0.51 |
| 24:YA:2096:U:O4 | 24:YA:2193:G:O6 | 2.28 | 0.51 |
| 24:YA:380:U:H2' | 24:YA:381:G:C8 | 2.45 | 0.51 |
| 24:YA:503:A:H4' | 24:YA:504:U:H5' | 1.93 | 0.51 |
| 27:YE:48:GLN:OE1 | 27:YE:64:LYS:NZ | 2.42 | 0.51 |
| 36:YR:24:GLN:HE22 | 36:YR:40:LYS:HB3 | 1.76 | 0.51 |
| 24:RA:2126:A:H4' | 24:RA:2127:G:O5' | 2.11 | 0.51 |
| 24:RA:2564:A:OP1 | 24:RA:2648:C:H4' | 2.11 | 0.51 |
| 24:RA:949:C:H2' | 24:RA:950:G:C8 | 2.46 | 0.51 |
| 30:RH:39:PRO:O | 30:RH:42:ARG:NH2 | 2.36 | 0.51 |
| 42:RX:27:THR:HB | 42:RX:80:ILE:HG12 | 1.93 | 0.51 |
| 1:XA:73:G:H1 | 1:XA:97:U:H3 | 1.58 | 0.51 |
| 20:XT:53:LEU:HA | 20:XT:56:MET:HG2 | 1.93 | 0.51 |
| 24:YA:2108:C:O2 | 24:YA:2181:G:N2 | 2.32 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:YA:303:U:H2' | 24:YA:304:G:H8 | 1.75 | 0.51 |
| 25:YB:15:A:H5' | 25:YB:16:G:C8 | 2.45 | 0.51 |
| 35:YQ:30:GLY:HA2 | 35:YQ:107:ALA:HB2 | 1.91 | 0.51 |
| 1:QA:1527:C:H2' | 1:QA:1528:U:C6 | 2.46 | 0.51 |
| 3:QC:10:PHE:HD1 | 3:QC:11:ARG:HD2 | 1.75 | 0.51 |
| 12:QL:113:ARG:HH21 | 12:QL:116:SER:HB2 | 1.76 | 0.51 |
| 24:RA:2052:G:H4' | 27:RE:143:ASN:O | 2.11 | 0.51 |
| 24:RA:2070:G:H2' | 24:RA:2071:A:C8 | 2.46 | 0.51 |
| 24:RA:962:G:H2' | 24:RA:963:U:C6 | 2.45 | 0.51 |
| 34:RP:52:GLU:HB2 | 34:RP:57:THR:HG22 | 1.92 | 0.51 |
| 1:XA:123:C:OP1 | 1:XA:311:C:O2' | 2.28 | 0.51 |
| 1:XA:671:G:O2' | 6:XF:80:ARG:NH1 | 2.41 | 0.51 |
| 1:XA:877:C:H2' | 1:XA:878:G:H8 | 1.74 | 0.51 |
| 22:XV:36:G:H2' | 22:XV:37:G:C8 | 2.46 | 0.51 |
| 24:YA:1113:U:H2' | 24:YA:1114:G:C8 | 2.46 | 0.51 |
| 24:YA:1416:G:H2' | 24:YA:1417:C:C6 | 2.46 | 0.51 |
| 24:YA:1464:C:HO2' | 24:YA:1528:A:H8 | 1.57 | 0.51 |
| 24:YA:2345:G:C6 | 24:YA:2347:C:N4 | 2.78 | 0.51 |
| 31:YI:39:ALA:HB1 | 31:YI:44:LEU:HD21 | 1.92 | 0.51 |
| 35:YQ:27:VAL:HG11 | 35:YQ:134:ARG:HA | 1.92 | 0.51 |
| 1:QA:1355:G:H2' | 1:QA:1356:G:C8 | 2.46 | 0.51 |
| 1:QA:902:G:H2' | 1:QA:903:G:H8 | 1.76 | 0.51 |
| 11:QK:34:ASP:HB3 | 11:QK:40:ILE:HD11 | 1.91 | 0.51 |
| 1:QA:195:A:H4' | 20:QT:68:LYS:HE3 | 1.91 | 0.51 |
| 24:RA:1353:A:H2' | 24:RA:1354:A:C8 | 2.46 | 0.51 |
| 24:RA:2122:U:H2' | 24:RA:2123:G:C8 | 2.46 | 0.51 |
| 24:RA:947:G:H2' | 24:RA:948:G:H8 | 1.76 | 0.51 |
| 27:RE:38:THR:OG1 | 27:RE:40:GLU:OE1 | 2.29 | 0.51 |
| 32:RN:47:ALA:HB2 | 32:RN:112:LEU:HD11 | 1.90 | 0.51 |
| 1:XA:1469:G:H2' | 1:XA:1470:G:H8 | 1.74 | 0.51 |
| 1:XA:723:U:OP1 | 23:XX:7:G:O2' | 2.28 | 0.51 |
| 24:YA:34:C:H41 | 24:YA:447:A:H61 | 1.58 | 0.51 |
| 24:YA:627:A:H4' | 24:YA:628:G:H5' | 1.91 | 0.51 |
| 24:YA:659:C:H2' | 24:YA:660:G:H8 | 1.74 | 0.51 |
| 36:YR:88:ARG:NH2 | 36:YR:89:ASP:OD1 | 2.44 | 0.51 |
| 1:QA:1151:A:H2' | 1:QA:1152:A:C8 | 2.46 | 0.51 |
| 2:QB:102:LEU:HD21 | 2:QB:182:ILE:HG13 | 1.93 | 0.51 |
| 8:QH:9:MET:O | 8:QH:13:ILE:HG12 | 2.11 | 0.51 |
| 13:QM:117:VAL:HG12 | 13:QM:118:ALA:H | 1.76 | 0.51 |
| 24:RA:2443:C:H2' | 24:RA:2444:G:H8 | 1.76 | 0.51 |
| 24:RA:2676:C:O2 | 24:RA:2732:G:N2 | 2.42 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:RG:124:SER:HB3 | 29:RG:131:TYR:HE2 | 1.76 | 0.51 |
| 43:RY:97:ARG:HG3 | 43:RY:106:LEU:HB2 | 1.93 | 0.51 |
| 2:XB:21:ARG:HB2 | 2:XB:39:ILE:HD13 | 1.93 | 0.51 |
| 4:XD:43:HIS:HA | 4:XD:46:LYS:HD3 | 1.93 | 0.51 |
| 24:YA:2354:G:H4' | 45:Y0:35:ASN:HD22 | 1.76 | 0.51 |
| 24:YA:1942:C:OP2 | 24:YA:1943:U:O2' | 2.21 | 0.51 |
| 25:YB:15:A:H5' | 25:YB:16:G:H8 | 1.76 | 0.51 |
| 29:YG:82:LEU:HD21 | 29:YG:88:ILE:HD13 | 1.92 | 0.51 |
| 31:YI:86:THR:HA | 31:YI:123:LEU:HB2 | 1.93 | 0.51 |
| 35:YQ:59:ARG:H | 35:YQ:59:ARG:HD2 | 1.75 | 0.51 |
| 1:QA:1032(B):G:N2 | 1:QA:1033:G:O6 | 2.43 | 0.51 |
| 1:QA:1175:G:H2' | 1:QA:1176:A:H8 | 1.76 | 0.51 |
| 1:QA:448:A:H62 | 1:QA:486:U:H3 | 1.58 | 0.51 |
| 10:QJ:54:PHE:CD2 | 10:QJ:55:LYS:HD3 | 2.46 | 0.51 |
| 22:QV:37:G:H2' | 22:QV:38:G:C8 | 2.46 | 0.51 |
| 24:RA:586:A:H5' | 28:RF:89:VAL:HG21 | 1.93 | 0.51 |
| 36:RR:104:ARG:HG3 | 36:RR:107:ASP:HB3 | 1.92 | 0.51 |
| 1:XA:1028:C:H2' | 1:XA:1028(A):C:C6 | 2.46 | 0.51 |
| 1:XA:689:C:OP2 | 11:XK:55:LYS:NZ | 2.44 | 0.51 |
| 1:XA:971:G:H5'' | 1:XA:972:C:H5'' | 1.91 | 0.51 |
| 49:Y4:26:SER:OG | 49:Y4:27:THR:N | 2.44 | 0.51 |
| 24:YA:2306:C:H2' | 24:YA:2307:G:H21 | 1.74 | 0.51 |
| 24:YA:576:U:H2' | 24:YA:577:G:C8 | 2.46 | 0.51 |
| 24:YA:2303:G:N3 | 29:YG:132:ASN:ND2 | 2.58 | 0.51 |
| 1:QA:701:C:OP1 | 1:QA:702:A:O2' | 2.20 | 0.51 |
| 1:QA:544:G:OP1 | 4:QD:59:ARG:NH2 | 2.44 | 0.51 |
| 12:QL:117:ARG:HB2 | 12:QL:122:THR:HB | 1.92 | 0.51 |
| 12:QL:58:VAL:HG11 | 12:QL:85:ILE:HD11 | 1.92 | 0.51 |
| 1:QA:1229:A:P | 13:QM:114:ARG:HH21 | 2.35 | 0.51 |
| 15:QO:54:ARG:HA | 15:QO:57:LEU:HD12 | 1.93 | 0.51 |
| 23:QX:6:C:H2' | 23:QX:7:A:C8 | 2.46 | 0.51 |
| 24:RA:1570:A:H2' | 24:RA:1571:A:C8 | 2.46 | 0.51 |
| 24:RA:2150:U:H2' | 24:RA:2151:G:H8 | 1.76 | 0.51 |
| 24:RA:221:A:H4' | 24:RA:222:A:O5' | 2.11 | 0.51 |
| 35:RQ:37:LEU:HD11 | 35:RQ:130:LYS:HB2 | 1.93 | 0.51 |
| 1:XA:558:G:OP2 | 1:XA:559:A:O2' | 2.25 | 0.51 |
| 1:XA:652:U:O4 | 1:XA:752:G:O2' | 2.22 | 0.51 |
| 4:XD:62:GLN:HE22 | 4:XD:65:ARG:HH21 | 1.59 | 0.51 |
| 24:YA:1139:G:O2' | 24:YA:1143:A:N1 | 2.39 | 0.51 |
| 24:YA:1265:A:H3' | 50:Y5:19:ARG:HH21 | 1.75 | 0.51 |
| 24:YA:1508:A:O2' | 24:YA:1509:C:O4' | 2.27 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:YA:1539:G:H2' | 24:YA:1540:G:C8 | 2.46 | 0.51 |
| 25:YB:37:C:O2 | 37:YS:95:HIS:NE2 | 2.41 | 0.51 |
| 1:QA:304:U:H2' | 1:QA:305:G:C8 | 2.47 | 0.50 |
| 1:QA:359:U:H2' | 1:QA:360:A:C8 | 2.47 | 0.50 |
| 1:QA:522:C:H41 | 12:QL:53:ARG:HH21 | 1.57 | 0.50 |
| 24:RA:1473:G:C8 | 24:RA:1473:G:C5' | 2.90 | 0.50 |
| 24:RA:1950:G:N2 | 24:RA:1950:G:OP2 | 2.35 | 0.50 |
| 24:RA:2749:A:H5'' | 30:RH:4:ILE:HD12 | 1.93 | 0.50 |
| 24:RA:181:A:H1' | 24:RA:435:C:H5' | 1.91 | 0.50 |
| 24:RA:530:G:O2' | 24:RA:532:A:N7 | 2.43 | 0.50 |
| 24:RA:662:G:H2' | 24:RA:663:G:H8 | 1.75 | 0.50 |
| 1:XA:1499:A:H1' | 1:XA:1520:G:H5' | 1.93 | 0.50 |
| 1:XA:484:G:H4' | 1:XA:485:G:O5' | 2.10 | 0.50 |
| 24:YA:1161:C:H2' | 24:YA:1162:G:H8 | 1.76 | 0.50 |
| 24:YA:1426:G:OP2 | 24:YA:1427:A:O2' | 2.20 | 0.50 |
| 35:YQ:77:LYS:NZ | 35:YQ:83:MET:O | 2.42 | 0.50 |
| 38:YT:118:ARG:HA | 38:YT:121:ILE:HG22 | 1.93 | 0.50 |
| 1:QA:701:C:H1' | 1:QA:703:G:C6 | 2.47 | 0.50 |
| 3:QC:116:VAL:HA | 3:QC:119:ARG:HG2 | 1.93 | 0.50 |
| 14:QN:24:CYS:HB3 | 14:QN:29:ARG:H | 1.76 | 0.50 |
| 1:QA:657:G:H4' | 15:QO:28:GLN:HG2 | 1.92 | 0.50 |
| 24:RA:1827:C:OP2 | 26:RD:222:ARG:NH1 | 2.44 | 0.50 |
| 24:RA:2368:C:H2' | 24:RA:2369:A:H8 | 1.75 | 0.50 |
| 24:RA:2441:C:OP2 | 24:RA:2586:C:O2' | 2.27 | 0.50 |
| 29:RG:37:VAL:H | 29:RG:99:MET:HE3 | 1.77 | 0.50 |
| 24:RA:270(L):U:H2' | 31:RI:50:ARG:HH12 | 1.76 | 0.50 |
| 1:XA:287:U:H2' | 1:XA:288:A:C8 | 2.47 | 0.50 |
| 1:XA:339:C:OP2 | 33:YO:97:ARG:HD3 | 2.10 | 0.50 |
| 8:XH:135:CYS:SG | 8:XH:136:GLU:N | 2.84 | 0.50 |
| 49:Y4:55:ARG:HD2 | 49:Y4:55:ARG:H | 1.76 | 0.50 |
| 24:YA:1292:U:H2' | 24:YA:1293:C:C6 | 2.47 | 0.50 |
| 24:YA:270(F):U:H3 | 24:YA:270(T):G:H1 | 1.60 | 0.50 |
| 24:YA:922:U:H2' | 24:YA:923:C:C6 | 2.47 | 0.50 |
| 25:YB:50:G:OP1 | 37:YS:63:THR:HG23 | 2.12 | 0.50 |
| 1:QA:973:G:O6 | 1:QA:974:A:N6 | 2.44 | 0.50 |
| 4:QD:63:LYS:O | 4:QD:67:ILE:HG13 | 2.10 | 0.50 |
| 4:QD:62:GLN:HE22 | 4:QD:65:ARG:HH21 | 1.60 | 0.50 |
| 22:QV:37:G:H2' | 22:QV:38:G:H8 | 1.75 | 0.50 |
| 24:RA:1830:C:H2' | 24:RA:1831:G:H8 | 1.76 | 0.50 |
| 24:RA:946:G:O6 | 24:RA:972:G:N2 | 2.45 | 0.50 |
| 43:RY:39:VAL:HG23 | 43:RY:42:VAL:HB | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:1273:G:H3' | 1:XA:1274:G:H8 | 1.74 | 0.50 |
| 1:XA:627:G:H2' | 1:XA:628:G:H8 | 1.76 | 0.50 |
| 24:YA:1000:A:H2' | 24:YA:1001:A:C8 | 2.46 | 0.50 |
| 24:YA:2103:C:O2 | 24:YA:2187:G:N2 | 2.44 | 0.50 |
| 24:YA:2115:G:O5' | 24:YA:2166:G:O2' | 2.29 | 0.50 |
| 24:YA:2776:A:H4' | 24:YA:2777:G:O5' | 2.10 | 0.50 |
| 8:QH:32:LYS:O | 8:QH:36:LEU:HG | 2.12 | 0.50 |
| 11:QK:44:SER:OG | 11:QK:45:GLY:N | 2.45 | 0.50 |
| 24:RA:83:G:O2' | 24:RA:102:G:N2 | 2.44 | 0.50 |
| 24:RA:1791:A:H3' | 24:RA:1792:G:H8 | 1.75 | 0.50 |
| 24:RA:2285:C:OP1 | 51:R6:29:ASN:ND2 | 2.45 | 0.50 |
| 24:RA:679:C:H2' | 24:RA:680:G:C8 | 2.46 | 0.50 |
| 38:RT:50:ILE:HD11 | 38:RT:100:TYR:HA | 1.92 | 0.50 |
| 1:XA:825:G:O2' | 8:XH:12:ARG:NH2 | 2.41 | 0.50 |
| 49:Y4:16:CYS:SG | 49:Y4:17:GLY:N | 2.84 | 0.50 |
| 24:YA:1203:G:H3' | 24:YA:1204:A:H5'' | 1.91 | 0.50 |
| 24:YA:1204:A:O2' | 24:YA:1205:U:O5' | 2.30 | 0.50 |
| 24:YA:2537:U:H2' | 24:YA:2538:C:C6 | 2.46 | 0.50 |
| 24:YA:531:C:OP1 | 24:YA:561:G:N1 | 2.44 | 0.50 |
| 24:YA:691:C:H2' | 24:YA:692:C:H6 | 1.77 | 0.50 |
| 44:YZ:4:ARG:HG2 | 44:YZ:58:VAL:HB | 1.93 | 0.50 |
| 1:QA:1031:G:H2' | 1:QA:1032:A:H8 | 1.77 | 0.50 |
| 1:QA:1326:C:OP1 | 21:QU:17:THR:OG1 | 2.30 | 0.50 |
| 49:R4:16:CYS:HB3 | 49:R4:20:ASN:HB3 | 1.93 | 0.50 |
| 24:RA:1527:G:N2 | 24:RA:1546:C:N3 | 2.59 | 0.50 |
| 24:RA:1826:G:OP1 | 26:RD:224:ALA:N | 2.43 | 0.50 |
| 24:RA:242:G:O2' | 24:RA:254:G:O6 | 2.28 | 0.50 |
| 1:XA:1412:C:H2' | 1:XA:1413:A:C8 | 2.47 | 0.50 |
| 14:YN:24:CYS:SG | 14:YN:29:ARG:HB3 | 2.52 | 0.50 |
| 24:YA:1570:A:H2' | 24:YA:1571:A:C8 | 2.46 | 0.50 |
| 24:YA:815:C:OP2 | 40:YV:83:ARG:NH1 | 2.44 | 0.50 |
| 31:YI:63:ALA:O | 31:YI:66:GLU:HG2 | 2.12 | 0.50 |
| 35:YQ:28:ALA:HB3 | 35:YQ:67:ARG:HH12 | 1.75 | 0.50 |
| 39:YU:90:VAL:HG12 | 39:YU:91:ASP:H | 1.76 | 0.50 |
| 44:YZ:13:GLU:HB3 | 44:YZ:18:LEU:HD21 | 1.93 | 0.50 |
| 1:QA:166:G:H2' | 1:QA:167:G:H8 | 1.77 | 0.50 |
| 1:QA:359:U:H2' | 1:QA:360:A:H8 | 1.77 | 0.50 |
| 1:QA:736:C:H2' | 1:QA:737:A:H8 | 1.75 | 0.50 |
| 1:QA:922:G:H2' | 1:QA:923:A:C8 | 2.46 | 0.50 |
| 1:QA:933:G:O6 | 7:QG:3:ARG:NH2 | 2.45 | 0.50 |
| 24:RA:1728:G:H8 | 24:RA:1732:A:H62 | 1.58 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:RG:140:ILE:HG13 | 29:RG:141:PHE:HD2 | 1.76 | 0.50 |
| 33:RO:2:ILE:HB | 33:RO:33:ALA:HB3 | 1.94 | 0.50 |
| 14:XN:24:CYS:SG | 14:XN:27:CYS:SG | 3.09 | 0.50 |
| 24:YA:2591:C:H2' | 24:YA:2592:G:H8 | 1.76 | 0.50 |
| 24:YA:2849:U:O4 | 38:YT:23:ARG:NH1 | 2.38 | 0.50 |
| 24:YA:358:U:H2' | 24:YA:359:A:H8 | 1.75 | 0.50 |
| 24:YA:428:A:H3' | 24:YA:429:A:H8 | 1.76 | 0.50 |
| 24:YA:510:C:H2' | 24:YA:511:U:O4' | 2.11 | 0.50 |
| 24:YA:847:U:O4 | 24:YA:933:A:N1 | 2.44 | 0.50 |
| 25:YB:5:C:OP1 | 25:YB:61:G:O2' | 2.29 | 0.50 |
| 27:YE:52:LEU:O | 27:YE:74:PRO:HA | 2.11 | 0.50 |
| 29:YG:16:ARG:HH21 | 29:YG:28:VAL:HG12 | 1.76 | 0.50 |
| 1:QA:1074:G:O2' | 2:QB:103:THR:OG1 | 2.23 | 0.50 |
| 1:QA:1200:C:O2' | 1:QA:1201:A:OP2 | 2.27 | 0.50 |
| 1:QA:514:C:H2' | 1:QA:515:G:C8 | 2.45 | 0.50 |
| 2:QB:136:VAL:HG23 | 2:QB:139:LYS:HE3 | 1.94 | 0.50 |
| 24:RA:582:G:H2' | 24:RA:583:G:H8 | 1.76 | 0.50 |
| 30:RH:4:ILE:HB | 30:RH:6:ARG:HH11 | 1.77 | 0.50 |
| 23:XX:1:G:H2' | 23:XX:2:G:H8 | 1.77 | 0.50 |
| 24:YA:1324:G:H1' | 24:YA:1616:A:N6 | 2.26 | 0.50 |
| 24:YA:271(D):G:H2' | 24:YA:272:G:H8 | 1.77 | 0.50 |
| 24:YA:828:U:H4' | 24:YA:831:G:C6 | 2.46 | 0.50 |
| 24:YA:1035:U:OP1 | 30:YH:59:ARG:NH1 | 2.45 | 0.50 |
| 1:QA:643:C:H5' | 8:QH:31:PHE:CD2 | 2.46 | 0.50 |
| 3:QC:113:ALA:HA | 3:QC:116:VAL:HG22 | 1.94 | 0.50 |
| 8:QH:111:ILE:HG23 | 8:QH:134:ILE:HB | 1.94 | 0.50 |
| 49:R4:51:ASP:HB2 | 49:R4:53:GLU:HG3 | 1.94 | 0.50 |
| 24:RA:1333:C:H2' | 24:RA:1334:G:H8 | 1.77 | 0.50 |
| 24:RA:1598:C:O3' | 42:RX:35:THR:OG1 | 2.30 | 0.50 |
| 24:RA:2056:G:N2 | 50:R5:4:HIS:O | 2.45 | 0.50 |
| 37:RS:110:LEU:HD12 | 37:RS:112:PHE:H | 1.77 | 0.50 |
| 27:RE:14:ILE:HG13 | 38:RT:14:TYR:HE2 | 1.77 | 0.50 |
| 1:XA:323:U:OP1 | 20:XT:26:ASN:ND2 | 2.45 | 0.50 |
| 1:XA:501:C:H1' | 1:XA:549:C:H1' | 1.92 | 0.50 |
| 1:XA:589:C:H5'' | 8:XH:29:SER:HB2 | 1.94 | 0.50 |
| 1:XA:997:U:H2' | 1:XA:998:G:C8 | 2.46 | 0.50 |
| 1:XA:1318:A:H1' | 19:XS:37:ARG:HH21 | 1.76 | 0.50 |
| 24:YA:1592:C:H2' | 24:YA:1593:G:C8 | 2.45 | 0.50 |
| 24:YA:1937:A:N7 | 24:YA:1939:U:H2' | 2.26 | 0.50 |
| 24:YA:1889:A:N3 | 24:YA:2086:U:O2' | 2.45 | 0.50 |
| 24:YA:288:C:H2' | 24:YA:289:A:C8 | 2.43 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1147:C:O2 | 9:QI:16:ARG:NH1 | 2.44 | 0.50 |
| 24:RA:1000:A:OP2 | 24:RA:1154:G:N1 | 2.24 | 0.50 |
| 24:RA:2183:C:H2' | 24:RA:2184:G:C8 | 2.46 | 0.50 |
| 24:RA:226:G:O2' | 24:RA:228:A:N6 | 2.44 | 0.50 |
| 24:RA:251:A:OP1 | 53:R8:7:HIS:NE2 | 2.30 | 0.50 |
| 26:RD:139:GLY:H | 26:RD:165:ILE:HG23 | 1.76 | 0.50 |
| 1:XA:1512:U:H2' | 1:XA:1513:A:C8 | 2.47 | 0.50 |
| 1:XA:256:U:OP1 | 17:XQ:17:LYS:NZ | 2.45 | 0.50 |
| 1:XA:483:C:OP2 | 1:XA:484:G:O2' | 2.23 | 0.50 |
| 1:XA:737:A:H2' | 1:XA:738:C:C6 | 2.47 | 0.50 |
| 24:YA:1230:C:H2' | 24:YA:1231:G:C8 | 2.47 | 0.50 |
| 24:YA:796:C:H2' | 24:YA:797:C:C6 | 2.47 | 0.50 |
| 33:YO:88:ASN:OD1 | 33:YO:92:GLU:N | 2.36 | 0.50 |
| 37:YS:26:LEU:HB3 | 37:YS:87:PHE:HA | 1.93 | 0.50 |
| 4:QD:119:GLN:HA | 4:QD:122:ARG:HE | 1.76 | 0.49 |
| 11:QK:29:ILE:HG22 | 11:QK:44:SER:HB2 | 1.93 | 0.49 |
| 24:RA:1629:U:H2' | 24:RA:1630:G:C8 | 2.47 | 0.49 |
| 28:RF:161:GLU:OE2 | 28:RF:164:ARG:NH2 | 2.42 | 0.49 |
| 43:RY:102:CYS:SG | 43:RY:103:GLY:N | 2.85 | 0.49 |
| 1:XA:112:G:H4' | 1:XA:389:A:H4' | 1.94 | 0.49 |
| 1:XA:1291:G:O2' | 9:XI:38:GLN:OE1 | 2.30 | 0.49 |
| 10:XJ:43:ARG:O | 10:XJ:67:THR:OG1 | 2.29 | 0.49 |
| 24:YA:2361:A:O5' | 53:Y8:27:THR:OG1 | 2.30 | 0.49 |
| 24:YA:2849:U:OP2 | 38:YT:95:ARG:NH1 | 2.44 | 0.49 |
| 24:YA:819:A:OP2 | 24:YA:1187:G:N2 | 2.40 | 0.49 |
| 25:YB:40:U:H3 | 25:YB:43:C:H5'' | 1.77 | 0.49 |
| 26:YD:148:GLU:OE1 | 26:YD:151:LYS:NZ | 2.44 | 0.49 |
| 32:YN:128:HIS:CE1 | 32:YN:134:ARG:HD2 | 2.47 | 0.49 |
| 1:QA:403:C:OP2 | 4:QD:74:GLN:NE2 | 2.45 | 0.49 |
| 1:QA:629:G:H2' | 1:QA:630:G:C8 | 2.47 | 0.49 |
| 3:QC:83:ARG:O | 3:QC:87:LEU:HG | 2.11 | 0.49 |
| 24:RA:308:G:HO2' | 24:RA:329:G:N2 | 2.08 | 0.49 |
| 24:RA:414:C:H2' | 24:RA:415:A:H8 | 1.77 | 0.49 |
| 24:RA:996:A:OP2 | 39:RU:92:ARG:NH2 | 2.46 | 0.49 |
| 1:XA:1306:A:N6 | 1:XA:1331:G:O2' | 2.46 | 0.49 |
| 1:XA:1409:C:H2' | 1:XA:1410:G:H8 | 1.77 | 0.49 |
| 1:XA:851:G:H2' | 1:XA:852:G:H8 | 1.77 | 0.49 |
| 7:XG:107:ALA:O | 7:XG:110:GLN:NE2 | 2.45 | 0.49 |
| 24:YA:151:C:H2' | 24:YA:152:G:H8 | 1.77 | 0.49 |
| 24:YA:1598:C:H5' | 42:YX:36:LYS:HB2 | 1.94 | 0.49 |
| 24:YA:2064:C:H2' | 24:YA:2065:C:C6 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:YA:597:U:H2' | 24:YA:598:G:C8 | 2.46 | 0.49 |
| 42:YX:26:TYR:HE2 | 42:YX:89:ILE:H | 1.60 | 0.49 |
| 44:YZ:7:ALA:HB2 | 44:YZ:59:LEU:HB3 | 1.94 | 0.49 |
| 1:QA:1129:C:H42 | 1:QA:1141:C:H41 | 1.60 | 0.49 |
| 1:QA:269:C:H2' | 1:QA:270:A:H8 | 1.77 | 0.49 |
| 4:QD:11:LEU:H | 4:QD:11:LEU:HD12 | 1.77 | 0.49 |
| 5:QE:121:LYS:NZ | 5:QE:122:GLU:O | 2.44 | 0.49 |
| 8:QH:51:VAL:HG21 | 8:QH:60:ARG:HG3 | 1.94 | 0.49 |
| 10:QJ:35:SER:HB2 | 10:QJ:73:ASP:HB2 | 1.93 | 0.49 |
| 24:RA:1216:G:OP1 | 39:RU:11:ARG:NH2 | 2.28 | 0.49 |
| 24:RA:1265:A:OP1 | 24:RA:1265:A:H8 | 1.94 | 0.49 |
| 24:RA:1780:A:O2' | 24:RA:1781:C:O2 | 2.24 | 0.49 |
| 24:RA:2056:G:OP2 | 24:RA:2057:A:OP2 | 2.30 | 0.49 |
| 24:RA:730:C:H3' | 24:RA:730:C:C6 | 2.47 | 0.49 |
| 24:RA:192:C:O2' | 24:RA:802:A:N3 | 2.42 | 0.49 |
| 24:RA:863:A:H2' | 24:RA:864:G:H8 | 1.77 | 0.49 |
| 36:RR:88:ARG:NH2 | 36:RR:89:ASP:OD1 | 2.45 | 0.49 |
| 37:RS:24:LEU:HB2 | 37:RS:85:VAL:HG13 | 1.94 | 0.49 |
| 1:XA:99:C:H2' | 1:XA:101:A:C8 | 2.47 | 0.49 |
| 24:YA:1779:U:OP2 | 24:YA:1784:A:N6 | 2.39 | 0.49 |
| 24:YA:1827:C:OP2 | 26:YD:222:ARG:NH1 | 2.42 | 0.49 |
| 24:YA:2008:C:H2' | 24:YA:2009:G:H8 | 1.76 | 0.49 |
| 25:YB:24:G:H1' | 25:YB:27:C:H41 | 1.78 | 0.49 |
| 29:YG:81:LYS:HD3 | 29:YG:86:MET:HE1 | 1.94 | 0.49 |
| 1:QA:662:G:O2' | 1:QA:836:G:OP1 | 2.30 | 0.49 |
| 10:QJ:16:LEU:HD12 | 10:QJ:94:VAL:HG22 | 1.95 | 0.49 |
| 1:QA:1302:U:O2 | 13:QM:27:LYS:NZ | 2.43 | 0.49 |
| 24:RA:1771:C:H2' | 24:RA:1772:G:C8 | 2.46 | 0.49 |
| 24:RA:2151:G:H2' | 24:RA:2152:G:H8 | 1.77 | 0.49 |
| 26:RD:148:GLU:OE1 | 26:RD:151:LYS:NZ | 2.40 | 0.49 |
| 27:RE:21:VAL:HG23 | 27:RE:185:LYS:HE3 | 1.94 | 0.49 |
| 2:XB:84:GLU:OE2 | 2:XB:233:SER:OG | 2.26 | 0.49 |
| 11:XK:34:ASP:OD1 | 11:XK:38:ASN:N | 2.45 | 0.49 |
| 24:YA:1399:C:H2' | 24:YA:1400:G:H8 | 1.76 | 0.49 |
| 24:YA:2468:G:O2' | 24:YA:2481:G:N2 | 2.46 | 0.49 |
| 24:YA:780:G:H21 | 24:YA:783:A:H62 | 1.60 | 0.49 |
| 24:RA:631:A:OP2 | 53:R8:46:ARG:NH2 | 2.46 | 0.49 |
| 24:RA:1286:A:O2' | 24:RA:1288:U:OP2 | 2.23 | 0.49 |
| 24:RA:1341:U:OP2 | 24:RA:1394:U:O2' | 2.26 | 0.49 |
| 24:RA:447:A:O4' | 24:RA:449:A:N6 | 2.46 | 0.49 |
| 24:RA:2495:G:H5'' | 35:RQ:81:VAL:HG12 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:XA:946:A:H2' | 1:XA:947:G:H8 | 1.78 | 0.49 |
| 2:XB:91:PRO:HG3 | 2:XB:154:LEU:HB2 | 1.95 | 0.49 |
| 3:XC:116:VAL:HG13 | 3:XC:140:ARG:HH21 | 1.77 | 0.49 |
| 7:XG:41:ARG:HH12 | 7:XG:115:ARG:HH21 | 1.60 | 0.49 |
| 8:XH:112:LEU:HG | 8:XH:133:LEU:HA | 1.94 | 0.49 |
| 10:XJ:30:SER:OG | 10:XJ:30:SER:O | 2.29 | 0.49 |
| 24:YA:2133:G:O2' | 24:YA:2158:A:N1 | 2.45 | 0.49 |
| 24:YA:822:U:H2' | 24:YA:823:G:H8 | 1.77 | 0.49 |
| 29:YG:31:VAL:O | 29:YG:33:ARG:NH1 | 2.43 | 0.49 |
| 1:QA:1112:C:H1' | 3:QC:179:ARG:HH11 | 1.78 | 0.49 |
| 1:QA:636:U:H2' | 1:QA:637:G:H8 | 1.78 | 0.49 |
| 24:RA:1426:G:OP2 | 24:RA:1427:A:O2' | 2.16 | 0.49 |
| 24:RA:1592:C:H2' | 24:RA:1593:G:H8 | 1.76 | 0.49 |
| 24:RA:1821:A:H2' | 24:RA:1822:G:C8 | 2.48 | 0.49 |
| 24:RA:2102:U:H2' | 24:RA:2103:C:H6 | 1.77 | 0.49 |
| 24:RA:2506:U:H3 | 24:RA:2584:U:H5 | 1.59 | 0.49 |
| 30:RH:25:LYS:HZ2 | 30:RH:27:LYS:H | 1.61 | 0.49 |
| 38:RT:3:ARG:HG3 | 38:RT:6:LEU:HB3 | 1.93 | 0.49 |
| 44:RZ:144:LEU:HD22 | 44:RZ:150:LEU:HG | 1.94 | 0.49 |
| 1:XA:816:A:OP2 | 1:XA:1526:G:O2' | 2.30 | 0.49 |
| 1:XA:673:G:O3' | 6:XF:87:ARG:NH2 | 2.46 | 0.49 |
| 24:YA:1645:G:H5'' | 24:YA:1646:C:C5' | 2.43 | 0.49 |
| 24:YA:2036:C:H2' | 24:YA:2037:G:H8 | 1.77 | 0.49 |
| 24:YA:2314:C:H2' | 24:YA:2315:G:C8 | 2.47 | 0.49 |
| 24:YA:2737:G:H2' | 24:YA:2738:A:C8 | 2.47 | 0.49 |
| 24:YA:969:U:H2' | 24:YA:970:C:C6 | 2.47 | 0.49 |
| 37:YS:20:ARG:NH1 | 45:Y0:48:GLY:O | 2.45 | 0.49 |
| 1:QA:1392:G:H21 | 1:QA:1502:A:H8 | 1.59 | 0.49 |
| 1:QA:707:C:H2' | 1:QA:708:C:C6 | 2.47 | 0.49 |
| 1:QA:362:G:OP2 | 12:QL:34:ARG:NH2 | 2.46 | 0.49 |
| 15:QO:76:GLU:OE2 | 15:QO:79:ARG:NH2 | 2.45 | 0.49 |
| 24:RA:2798:C:H2' | 24:RA:2799:A:C8 | 2.47 | 0.49 |
| 24:RA:288:C:H2' | 24:RA:289:A:H8 | 1.77 | 0.49 |
| 24:RA:581:C:H2' | 24:RA:582:G:C8 | 2.47 | 0.49 |
| 24:RA:1657:C:HO2' | 27:RE:133:LYS:HD2 | 1.76 | 0.49 |
| 1:XA:1355:G:H2' | 1:XA:1356:G:H8 | 1.76 | 0.49 |
| 23:XX:3:C:H2' | 23:XX:4:A:C8 | 2.48 | 0.49 |
| 24:YA:1059:G:OP2 | 24:YA:1060:U:H5'' | 2.12 | 0.49 |
| 24:YA:2183:C:H2' | 24:YA:2184:G:H8 | 1.76 | 0.49 |
| 24:YA:2289:G:H2' | 24:YA:2290:G:H8 | 1.77 | 0.49 |
| 24:YA:2676:C:H2' | 24:YA:2677:G:H8 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:YA:2702:U:OP1 | 24:YA:2702:U:H6 | 1.96 | 0.49 |
| 24:YA:2836:U:H2' | 24:YA:2837:G:C8 | 2.47 | 0.49 |
| 24:YA:2884:U:H2' | 24:YA:2885:C:O4' | 2.12 | 0.49 |
| 29:YG:129:GLY:HA2 | 29:YG:166:ASP:HA | 1.94 | 0.49 |
| 8:QH:109:ILE:HD11 | 8:QH:120:THR:HB | 1.95 | 0.49 |
| 12:QL:46:LYS:HZ2 | 12:QL:47:LYS:H | 1.59 | 0.49 |
| 24:RA:2689:U:H4' | 24:RA:2690:C:O5' | 2.13 | 0.49 |
| 24:RA:840:C:H2' | 24:RA:841:A:H8 | 1.76 | 0.49 |
| 24:RA:922:U:H2' | 24:RA:923:C:C6 | 2.47 | 0.49 |
| 24:RA:1006:C:H5' | 32:RN:28:THR:HG23 | 1.95 | 0.49 |
| 43:RY:37:VAL:O | 43:RY:67:LEU:N | 2.42 | 0.49 |
| 1:XA:1004:A:H1' | 1:XA:1036:G:H22 | 1.77 | 0.49 |
| 1:XA:407:G:OP1 | 4:XD:115:ARG:NH1 | 2.46 | 0.49 |
| 4:XD:61:LYS:HD2 | 4:XD:206:PHE:CE2 | 2.48 | 0.49 |
| 5:XE:102:ALA:O | 5:XE:107:ARG:NH2 | 2.46 | 0.49 |
| 8:XH:83:ILE:HG22 | 8:XH:137:VAL:HG22 | 1.93 | 0.49 |
| 14:XN:3:ARG:HH21 | 14:XN:4:LYS:HD3 | 1.76 | 0.49 |
| 47:Y2:25:VAL:O | 47:Y2:29:LYS:HG2 | 2.12 | 0.49 |
| 24:YA:2627:G:O2' | 24:YA:2781:A:N1 | 2.34 | 0.49 |
| 24:YA:319:C:H2' | 24:YA:320:A:C8 | 2.48 | 0.49 |
| 24:YA:852:G:H2' | 24:YA:853:G:H8 | 1.78 | 0.49 |
| 37:YS:25:ARG:NH1 | 37:YS:42:ASP:OD2 | 2.46 | 0.49 |
| 1:QA:1251:A:H2' | 1:QA:1252:A:C8 | 2.48 | 0.49 |
| 4:QD:101:LEU:HD12 | 4:QD:138:TYR:HB3 | 1.94 | 0.49 |
| 5:QE:76:ILE:HG23 | 5:QE:142:LEU:HD13 | 1.95 | 0.49 |
| 12:QL:32:PHE:HB3 | 12:QL:84:LEU:HD11 | 1.94 | 0.49 |
| 42:RX:8:ILE:O | 47:R2:36:ARG:NH2 | 2.46 | 0.49 |
| 24:RA:1791:A:H5' | 26:RD:206:LEU:HD12 | 1.94 | 0.49 |
| 24:RA:2291:U:H2' | 24:RA:2292:C:C6 | 2.48 | 0.49 |
| 24:RA:303:U:H2' | 24:RA:304:G:H8 | 1.77 | 0.49 |
| 35:RQ:58:PHE:HD2 | 35:RQ:61:GLY:HA3 | 1.78 | 0.49 |
| 39:RU:61:TRP:HB3 | 39:RU:93:LYS:O | 2.12 | 0.49 |
| 44:RZ:53:ILE:HG22 | 44:RZ:71:VAL:HG13 | 1.93 | 0.49 |
| 1:XA:345:C:H1' | 1:XA:346:G:OP2 | 2.12 | 0.49 |
| 3:XC:157:ILE:HG22 | 3:XC:164:ARG:HH21 | 1.77 | 0.49 |
| 3:XC:182:ILE:HD11 | 3:XC:201:TYR:HB3 | 1.93 | 0.49 |
| 9:XI:5:TYR:HE1 | 9:XI:16:ARG:HB2 | 1.77 | 0.49 |
| 9:XI:73:GLN:O | 9:XI:77:ILE:HG12 | 2.13 | 0.49 |
| 10:XJ:7:LYS:HB3 | 10:XJ:97:GLU:HB3 | 1.94 | 0.49 |
| 17:XQ:28:PRO:HA | 17:XQ:35:VAL:HA | 1.95 | 0.49 |
| 23:XX:5:A:H2' | 23:XX:6:G:C8 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:YA:1580:A:H5' | 24:YA:1581:G:OP2 | 2.13 | 0.49 |
| 24:YA:1615:C:OP2 | 24:YA:1617:C:N4 | 2.33 | 0.49 |
| 24:YA:532:A:N1 | 24:YA:2035:G:N2 | 2.60 | 0.49 |
| 24:YA:2743:C:OP2 | 24:YA:2755:C:N4 | 2.46 | 0.49 |
| 24:YA:277:C:H5' | 24:YA:278:A:H5' | 1.95 | 0.49 |
| 24:YA:689:A:H2' | 24:YA:690:G:H8 | 1.78 | 0.49 |
| 26:YD:123:ALA:HB3 | 26:YD:131:LEU:HG | 1.95 | 0.49 |
| 24:YA:2294:C:OP2 | 37:YS:13:ARG:NH2 | 2.45 | 0.49 |
| 43:YY:48:ALA:HA | 43:YY:60:PHE:HD2 | 1.77 | 0.49 |
| 1:QA:1287:A:H2 | 1:QA:1353:G:H1' | 1.78 | 0.49 |
| 1:QA:1320:C:H42 | 19:QS:36:ARG:HB2 | 1.78 | 0.49 |
| 22:QV:44:G:H2' | 22:QV:45:G:C8 | 2.47 | 0.49 |
| 24:RA:2584:U:H2' | 24:RA:2585:U:H2' | 1.95 | 0.49 |
| 24:RA:270(I):G:H2' | 24:RA:270(J):G:C8 | 2.48 | 0.49 |
| 24:RA:86:C:H4' | 24:RA:104:U:H1' | 1.95 | 0.49 |
| 24:RA:969:U:H2' | 24:RA:970:C:C6 | 2.48 | 0.49 |
| 1:XA:1225:A:H5'' | 1:XA:1226:C:OP2 | 2.13 | 0.49 |
| 1:XA:524:G:H2' | 1:XA:525:C:C6 | 2.48 | 0.49 |
| 1:XA:628:G:H2' | 1:XA:629:G:C8 | 2.48 | 0.49 |
| 1:XA:708:C:H2' | 1:XA:709:G:H8 | 1.78 | 0.49 |
| 4:XD:88:VAL:HG22 | 4:XD:90:GLY:H | 1.77 | 0.49 |
| 13:XM:78:ILE:HD11 | 13:XM:92:HIS:HB3 | 1.94 | 0.49 |
| 21:XU:8:THR:HG23 | 21:XU:11:GLY:H | 1.78 | 0.49 |
| 49:Y4:34:GLU:HG2 | 49:Y4:35:VAL:HG12 | 1.93 | 0.49 |
| 24:YA:2355:C:H1' | 45:Y0:39:ARG:HH21 | 1.78 | 0.49 |
| 24:YA:607:U:H3 | 24:YA:621:A:H2 | 1.61 | 0.49 |
| 24:YA:259:G:H21 | 24:YA:621:A:H8 | 1.60 | 0.49 |
| 24:YA:2318:G:H22 | 37:YS:2:ALA:HA | 1.78 | 0.49 |
| 1:QA:924:C:O2' | 1:QA:1502:A:N6 | 2.46 | 0.48 |
| 1:QA:41:G:H2' | 1:QA:42:G:H8 | 1.77 | 0.48 |
| 1:QA:662:G:H2' | 1:QA:663:A:C8 | 2.48 | 0.48 |
| 20:QT:51:GLU:O | 20:QT:55:ILE:HG12 | 2.13 | 0.48 |
| 24:RA:640:C:H2' | 24:RA:641:C:C6 | 2.48 | 0.48 |
| 24:RA:784:A:OP2 | 24:RA:2589:A:OP1 | 2.30 | 0.48 |
| 40:RV:57:VAL:HG12 | 40:RV:99:ILE:HG23 | 1.94 | 0.48 |
| 1:XA:119:A:C8 | 1:XA:288:A:C6 | 3.01 | 0.48 |
| 1:XA:427:U:OP2 | 1:XA:428:G:O2' | 2.29 | 0.48 |
| 1:XA:191(G):G:C4 | 20:XT:105:SER:HB3 | 2.48 | 0.48 |
| 24:YA:2735:G:H2' | 24:YA:2736:G:H8 | 1.78 | 0.48 |
| 24:YA:2619:C:H5'' | 27:YE:152:LYS:HA | 1.95 | 0.48 |
| 32:YN:137:LYS:HD3 | 32:YN:138:LEU:N | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1075:C:H5'' | 2:QB:179:LYS:NZ | 2.28 | 0.48 |
| 1:QA:346:G:H1' | 1:QA:347:G:H5' | 1.95 | 0.48 |
| 24:RA:1593:G:H2' | 24:RA:1594:G:C8 | 2.47 | 0.48 |
| 24:RA:2197:U:H1' | 24:RA:2198:A:C8 | 2.48 | 0.48 |
| 24:RA:2469:A:H2' | 35:RQ:56:ARG:HE | 1.78 | 0.48 |
| 24:RA:270:A:OP2 | 24:RA:270(Y):G:N1 | 2.46 | 0.48 |
| 24:RA:2747:G:N2 | 24:RA:2757:A:H62 | 2.09 | 0.48 |
| 26:RD:90:ALA:HB3 | 26:RD:106:ILE:HD11 | 1.94 | 0.48 |
| 1:XA:309:G:H2' | 1:XA:310:G:H8 | 1.79 | 0.48 |
| 1:XA:41:G:H2' | 1:XA:42:G:H8 | 1.78 | 0.48 |
| 1:XA:693:G:H2' | 1:XA:694:A:C8 | 2.48 | 0.48 |
| 4:XD:158:ILE:O | 4:XD:162:LEU:HG | 2.13 | 0.48 |
| 7:XG:15:ASP:HB3 | 7:XG:19:GLY:H | 1.78 | 0.48 |
| 15:XO:70:LEU:HD21 | 15:XO:77:ARG:HG3 | 1.95 | 0.48 |
| 24:YA:1405:U:H2' | 24:YA:1406:U:C6 | 2.47 | 0.48 |
| 24:YA:1438:U:H2' | 24:YA:1439:A:H8 | 1.78 | 0.48 |
| 24:YA:1647:G:H3' | 24:YA:1647:G:OP2 | 2.14 | 0.48 |
| 24:YA:2655:G:N2 | 24:YA:2665:A:OP2 | 2.47 | 0.48 |
| 29:YG:136:ARG:HG2 | 29:YG:137:GLU:H | 1.78 | 0.48 |
| 1:QA:164:U:H2' | 1:QA:165:C:C6 | 2.48 | 0.48 |
| 1:QA:539:A:H2' | 1:QA:540:G:C8 | 2.48 | 0.48 |
| 2:QB:71:VAL:HA | 2:QB:93:VAL:HB | 1.95 | 0.48 |
| 9:QI:73:GLN:O | 9:QI:77:ILE:HG12 | 2.13 | 0.48 |
| 10:QJ:30:SER:HB2 | 10:QJ:80:LYS:HG3 | 1.94 | 0.48 |
| 16:QP:67:THR:HG22 | 16:QP:68:ASP:H | 1.78 | 0.48 |
| 24:RA:2306:C:H3' | 24:RA:2307:G:H5'' | 1.95 | 0.48 |
| 24:RA:2431:U:N3 | 24:RA:2434:A:OP2 | 2.32 | 0.48 |
| 24:RA:2581:G:OP2 | 24:RA:2581:G:N2 | 2.46 | 0.48 |
| 24:RA:2701:C:H3' | 24:RA:2702:U:C5' | 2.44 | 0.48 |
| 24:RA:479:A:HO2' | 24:RA:481:G:H8 | 1.60 | 0.48 |
| 33:RO:63:VAL:HG12 | 33:RO:106:LEU:HD21 | 1.94 | 0.48 |
| 34:RP:90:ARG:HG3 | 34:RP:91:PHE:HD1 | 1.79 | 0.48 |
| 38:RT:109:GLU:OE1 | 38:RT:112:ARG:NH1 | 2.46 | 0.48 |
| 19:XS:3:ARG:HH12 | 19:XS:11:VAL:HG22 | 1.77 | 0.48 |
| 1:XA:1230:C:H5' | 22:XV:31:C:H5'' | 1.95 | 0.48 |
| 46:Y1:46:LEU:O | 46:Y1:47:GLN:NE2 | 2.47 | 0.48 |
| 24:YA:1853:A:N3 | 24:YA:2233:U:O2' | 2.41 | 0.48 |
| 24:YA:1869:G:H5' | 24:YA:1870:C:OP2 | 2.13 | 0.48 |
| 24:YA:270(I):G:H2' | 24:YA:270(J):G:C8 | 2.47 | 0.48 |
| 24:YA:511:U:H5'' | 24:YA:1236:G:OP1 | 2.13 | 0.48 |
| 24:YA:675:A:N3 | 24:YA:2443:C:O2' | 2.39 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:YA:918:A:N3 | 25:YB:80:U:O2' | 2.44 | 0.48 |
| 26:YD:147:LEU:HD21 | 26:YD:183:ARG:HH22 | 1.78 | 0.48 |
| 1:QA:1043:C:H2' | 1:QA:1044:A:H8 | 1.77 | 0.48 |
| 1:QA:552:U:H2' | 1:QA:553:A:H8 | 1.78 | 0.48 |
| 1:QA:745:C:H2' | 1:QA:746:A:C8 | 2.48 | 0.48 |
| 1:QA:745:C:H2' | 1:QA:746:A:H8 | 1.78 | 0.48 |
| 8:QH:12:ARG:HD2 | 8:QH:26:VAL:HG22 | 1.94 | 0.48 |
| 24:RA:1525:G:H2' | 24:RA:1526:G:C8 | 2.48 | 0.48 |
| 24:RA:2452:C:H2' | 24:RA:2453:A:C8 | 2.48 | 0.48 |
| 24:RA:2737:G:H2' | 24:RA:2738:A:C8 | 2.47 | 0.48 |
| 24:RA:995:C:O2 | 32:RN:3:THR:OG1 | 2.32 | 0.48 |
| 1:XA:50:A:H1' | 1:XA:52:G:C8 | 2.48 | 0.48 |
| 1:XA:590:C:OP1 | 8:XH:30:ARG:N | 2.42 | 0.48 |
| 1:XA:748:C:H1' | 1:XA:749:C:H5 | 1.79 | 0.48 |
| 1:XA:877:C:H2' | 1:XA:878:G:C8 | 2.48 | 0.48 |
| 1:XA:430:A:P | 4:XD:8:VAL:H | 2.37 | 0.48 |
| 47:Y2:45:SER:O | 47:Y2:46:GLN:NE2 | 2.46 | 0.48 |
| 24:YA:1408:C:H2' | 24:YA:1409:C:C6 | 2.49 | 0.48 |
| 24:YA:1812:A:H2' | 24:YA:1813:G:H8 | 1.79 | 0.48 |
| 24:YA:2001:A:H2' | 24:YA:2002:G:C8 | 2.49 | 0.48 |
| 24:YA:210:C:H2' | 24:YA:211:A:H8 | 1.77 | 0.48 |
| 24:YA:587:C:OP2 | 34:YP:21:ARG:NH1 | 2.30 | 0.48 |
| 43:YY:47:LYS:NZ | 43:YY:48:ALA:O | 2.43 | 0.48 |
| 1:QA:1047:G:H5'' | 14:QN:4:LYS:HD2 | 1.96 | 0.48 |
| 1:QA:501:C:H2' | 1:QA:502:G:C8 | 2.48 | 0.48 |
| 1:QA:639:G:H2' | 1:QA:640:A:H8 | 1.77 | 0.48 |
| 12:QL:110:VAL:O | 12:QL:122:THR:OG1 | 2.28 | 0.48 |
| 22:QV:66:U:H2' | 22:QV:67:A:H8 | 1.79 | 0.48 |
| 29:RG:142:PRO:HB2 | 49:R4:31:ILE:HG21 | 1.95 | 0.48 |
| 24:RA:116:C:O2' | 24:RA:126:A:N3 | 2.42 | 0.48 |
| 24:RA:1411:C:H42 | 24:RA:1591:G:H1 | 1.62 | 0.48 |
| 24:RA:2514:U:H2' | 24:RA:2515:C:C6 | 2.48 | 0.48 |
| 24:RA:2698:U:H2' | 24:RA:2699:C:C6 | 2.48 | 0.48 |
| 24:RA:2784:C:O2' | 27:RE:37:ARG:NH1 | 2.46 | 0.48 |
| 24:RA:2787:C:H1' | 27:RE:62:PRO:HG3 | 1.94 | 0.48 |
| 37:RS:8:GLU:O | 37:RS:11:LYS:HB3 | 2.14 | 0.48 |
| 1:XA:17:U:H2' | 1:XA:18:C:C6 | 2.49 | 0.48 |
| 1:XA:343:U:O2 | 1:XA:346:G:N1 | 2.47 | 0.48 |
| 2:XB:76:GLN:HG2 | 2:XB:208:ILE:HG13 | 1.96 | 0.48 |
| 3:XC:83:ARG:O | 3:XC:87:LEU:HG | 2.14 | 0.48 |
| 24:YA:1939:U:H3' | 24:YA:1940:U:H5' | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:YA:2037:G:H2' | 24:YA:2038:G:C8 | 2.47 | 0.48 |
| 24:YA:2515:C:H2' | 24:YA:2516:G:H8 | 1.77 | 0.48 |
| 24:YA:2737:G:H2' | 24:YA:2738:A:H8 | 1.79 | 0.48 |
| 24:YA:848:G:H2' | 24:YA:849:A:C8 | 2.48 | 0.48 |
| 24:YA:956:G:OP2 | 35:YQ:14:ARG:NH2 | 2.46 | 0.48 |
| 28:YF:122:LYS:HB3 | 28:YF:191:ARG:HG3 | 1.94 | 0.48 |
| 34:YP:52:GLU:OE2 | 34:YP:58:THR:OG1 | 2.28 | 0.48 |
| 24:YA:1243:G:H4' | 34:YP:7:ARG:HH21 | 1.78 | 0.48 |
| 35:YQ:41:TRP:HB3 | 35:YQ:94:VAL:HG21 | 1.95 | 0.48 |
| 1:QA:563:A:O2' | 1:QA:566:G:O3' | 2.30 | 0.48 |
| 3:QC:157:ILE:HD13 | 3:QC:166:GLU:HG2 | 1.94 | 0.48 |
| 22:QV:59:A:O2' | 22:QV:61:U:OP2 | 2.16 | 0.48 |
| 23:QX:11:A:H2' | 23:QX:12:G:C8 | 2.48 | 0.48 |
| 29:RG:3:LEU:HD12 | 49:R4:25:TYR:HE2 | 1.79 | 0.48 |
| 24:RA:2627:G:N2 | 24:RA:2777:G:OP2 | 2.47 | 0.48 |
| 24:RA:271(D):G:H2' | 24:RA:272:G:C8 | 2.49 | 0.48 |
| 24:RA:271(D):G:H2' | 24:RA:272:G:H8 | 1.78 | 0.48 |
| 24:RA:2841:C:H2' | 24:RA:2842:G:H8 | 1.79 | 0.48 |
| 1:XA:1244:C:OP2 | 21:XU:9:ARG:NE | 2.47 | 0.48 |
| 24:YA:1754:C:OP1 | 38:YT:96:ARG:NH1 | 2.47 | 0.48 |
| 24:YA:2853:C:H2' | 24:YA:2854:G:H8 | 1.78 | 0.48 |
| 24:YA:363(B):G:H2' | 24:YA:363(C):G:H8 | 1.79 | 0.48 |
| 24:YA:578:A:OP1 | 24:YA:1255:U:O2' | 2.28 | 0.48 |
| 26:YD:17:THR:HG22 | 26:YD:204:ILE:HD12 | 1.95 | 0.48 |
| 26:YD:72:LYS:HG3 | 26:YD:97:TYR:CE2 | 2.48 | 0.48 |
| 27:YE:26:ILE:HB | 27:YE:182:LEU:HB3 | 1.95 | 0.48 |
| 29:YG:107:LEU:HD13 | 29:YG:111:LEU:HD12 | 1.96 | 0.48 |
| 30:YH:46:GLU:OE1 | 30:YH:51:ARG:NH1 | 2.47 | 0.48 |
| 1:QA:1151:A:H2' | 1:QA:1152:A:H8 | 1.79 | 0.48 |
| 1:QA:5:U:O2' | 1:QA:6:G:O5' | 2.32 | 0.48 |
| 4:QD:133:VAL:HG12 | 4:QD:135:LEU:H | 1.78 | 0.48 |
| 5:QE:75:THR:HA | 5:QE:115:VAL:HG13 | 1.95 | 0.48 |
| 7:QG:54:THR:HG22 | 7:QG:56:GLN:HG2 | 1.95 | 0.48 |
| 8:QH:36:LEU:HA | 8:QH:39:LEU:HD12 | 1.94 | 0.48 |
| 10:QJ:38:ILE:HD12 | 10:QJ:39:PRO:HD2 | 1.96 | 0.48 |
| 1:QA:1367:C:H5' | 10:QJ:60:ARG:NH1 | 2.28 | 0.48 |
| 24:RA:1295:C:H2' | 24:RA:1296:G:H8 | 1.79 | 0.48 |
| 24:RA:2466:C:OP1 | 54:R9:4:ARG:HB2 | 2.14 | 0.48 |
| 24:RA:463:G:N2 | 24:RA:466:A:OP2 | 2.32 | 0.48 |
| 24:RA:514:A:N3 | 24:RA:581:C:O2' | 2.39 | 0.48 |
| 25:RB:89:G:H2' | 25:RB:89(A):A:C8 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:RI:26:ALA:HA | 31:RI:30:LEU:HB2 | 1.95 | 0.48 |
| 37:RS:25:ARG:NH1 | 37:RS:42:ASP:OD2 | 2.46 | 0.48 |
| 1:XA:1291:G:H4' | 9:XI:39:GLY:HA3 | 1.95 | 0.48 |
| 54:Y9:25:VAL:HB | 54:Y9:34:GLN:HB2 | 1.95 | 0.48 |
| 24:YA:1403:C:H5'' | 24:YA:1471:A:H1' | 1.96 | 0.48 |
| 24:YA:2341:G:H2' | 24:YA:2342:C:C6 | 2.48 | 0.48 |
| 24:YA:1939:U:OP1 | 24:YA:2604:U:O2' | 2.32 | 0.48 |
| 24:YA:270(R):G:H2' | 24:YA:270(S):G:C8 | 2.48 | 0.48 |
| 39:YU:91:ASP:O | 39:YU:93:LYS:N | 2.47 | 0.48 |
| 1:QA:1314:C:OP2 | 19:QS:4:SER:OG | 2.20 | 0.48 |
| 1:QA:944:G:N1 | 1:QA:1338:G:OP2 | 2.44 | 0.48 |
| 1:QA:1435:G:H2' | 1:QA:1436:U:C6 | 2.49 | 0.48 |
| 1:QA:1446:A:O2' | 1:QA:1447:G:O5' | 2.24 | 0.48 |
| 3:QC:11:ARG:O | 3:QC:13:GLY:N | 2.47 | 0.48 |
| 7:QG:23:VAL:HG13 | 7:QG:43:PHE:HE2 | 1.79 | 0.48 |
| 7:QG:27:ILE:HA | 7:QG:30:ILE:HG22 | 1.96 | 0.48 |
| 24:RA:1546:C:H5' | 24:RA:1547:C:H5' | 1.95 | 0.48 |
| 25:RB:24:G:O6 | 25:RB:56:G:O2' | 2.27 | 0.48 |
| 33:RO:47:ILE:O | 33:RO:53:LYS:NZ | 2.47 | 0.48 |
| 34:RP:52:GLU:OE2 | 34:RP:58:THR:OG1 | 2.32 | 0.48 |
| 37:RS:109:GLY:O | 37:RS:110:LEU:HG | 2.14 | 0.48 |
| 37:RS:15:ARG:NE | 37:RS:88:ASP:OD1 | 2.46 | 0.48 |
| 3:XC:9:GLY:HA2 | 3:XC:12:LEU:HG | 1.96 | 0.48 |
| 3:XC:172:ARG:HG3 | 3:XC:174:PRO:HD3 | 1.94 | 0.48 |
| 7:XG:29:LYS:HG3 | 7:XG:105:VAL:HG11 | 1.96 | 0.48 |
| 24:YA:1794:U:H2' | 24:YA:1795:C:H6 | 1.78 | 0.48 |
| 24:YA:2420:C:H5' | 51:Y6:54:ILE:HD11 | 1.96 | 0.48 |
| 24:YA:746:A:HO2' | 24:YA:2611:U:HO2' | 1.56 | 0.48 |
| 28:YF:63:LYS:NZ | 28:YF:75:HIS:O | 2.39 | 0.48 |
| 1:QA:1407:C:H2' | 1:QA:1408:A:H8 | 1.78 | 0.48 |
| 1:QA:977:A:N6 | 1:QA:1224:G:OP1 | 2.47 | 0.48 |
| 13:QM:37:THR:HG21 | 13:QM:56:LEU:HA | 1.96 | 0.48 |
| 47:R2:10:LEU:HG | 47:R2:14:ARG:HE | 1.79 | 0.48 |
| 24:RA:1359:A:OP2 | 24:RA:1371:G:N2 | 2.43 | 0.48 |
| 24:RA:1416:G:H2' | 24:RA:1417:C:C6 | 2.49 | 0.48 |
| 24:RA:2707:G:H2' | 24:RA:2708:G:H8 | 1.78 | 0.48 |
| 4:XD:96:LEU:HD13 | 4:XD:139:ARG:HE | 1.79 | 0.48 |
| 10:XJ:84:GLN:HA | 10:XJ:88:LEU:HD13 | 1.96 | 0.48 |
| 11:XK:57:THR:HG22 | 11:XK:59:TYR:H | 1.79 | 0.48 |
| 24:YA:1252:G:N2 | 39:YU:37:GLU:OE2 | 2.44 | 0.48 |
| 24:YA:1754:C:N3 | 24:YA:2716:U:O2' | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:YA:2071:A:H2' | 24:YA:2072:G:H8 | 1.79 | 0.48 |
| 24:YA:270(H):C:H2' | 24:YA:270(I):G:C8 | 2.48 | 0.48 |
| 24:YA:2773:C:OP1 | 27:YE:164:ARG:NE | 2.40 | 0.48 |
| 24:YA:385:C:O2' | 24:YA:388:G:N2 | 2.47 | 0.48 |
| 25:YB:30:C:O2' | 25:YB:57:A:N1 | 2.45 | 0.48 |
| 29:YG:58:GLN:O | 29:YG:62:LEU:HG | 2.13 | 0.48 |
| 44:YZ:128:VAL:HG23 | 44:YZ:161:VAL:HG22 | 1.96 | 0.48 |
| 2:QB:169:LYS:NZ | 2:QB:191:ASP:OD2 | 2.46 | 0.48 |
| 2:QB:33:TYR:HB3 | 2:QB:41:ILE:HG13 | 1.95 | 0.48 |
| 24:RA:1590:U:H2' | 24:RA:1591:G:C8 | 2.49 | 0.48 |
| 24:RA:1651:G:H4' | 36:RR:39:PRO:HG2 | 1.95 | 0.48 |
| 24:RA:2642:G:H5' | 32:RN:78:TYR:CD2 | 2.49 | 0.48 |
| 24:RA:37:C:H2' | 24:RA:38:A:H8 | 1.79 | 0.48 |
| 26:RD:25:THR:HG22 | 26:RD:82:ILE:H | 1.78 | 0.48 |
| 30:RH:79:VAL:HG12 | 30:RH:136:ILE:HD11 | 1.96 | 0.48 |
| 44:RZ:54:HIS:HB3 | 44:RZ:101:PRO:HD3 | 1.95 | 0.48 |
| 1:XA:352:C:O2' | 1:XA:354:G:OP1 | 2.20 | 0.48 |
| 1:XA:656:C:O2 | 15:XO:28:GLN:NE2 | 2.45 | 0.48 |
| 14:YN:39:LEU:HD12 | 14:YN:44:LEU:HB3 | 1.95 | 0.48 |
| 17:XQ:4:LYS:NZ | 17:XQ:5:VAL:O | 2.46 | 0.48 |
| 18:XR:74:ARG:HD3 | 18:XR:81:PHE:HA | 1.96 | 0.48 |
| 24:YA:1186:G:H2' | 24:YA:1187:G:O4' | 2.14 | 0.48 |
| 1:QA:1024:G:OP1 | 1:QA:1024:G:H4' | 2.14 | 0.47 |
| 1:QA:559:A:H4' | 1:QA:560:U:H3' | 1.96 | 0.47 |
| 13:QM:31:LYS:HD3 | 13:QM:34:LEU:HD21 | 1.95 | 0.47 |
| 23:QX:8:A:H2' | 23:QX:9:G:C8 | 2.49 | 0.47 |
| 24:RA:1454:U:O2' | 24:RA:1455:G:N7 | 2.43 | 0.47 |
| 24:RA:1646:C:H5'' | 24:RA:1647:G:H5'' | 1.95 | 0.47 |
| 33:RO:88:ASN:OD1 | 33:RO:92:GLU:N | 2.39 | 0.47 |
| 1:XA:324:G:OP1 | 20:XT:22:ARG:NE | 2.46 | 0.47 |
| 1:XA:627:G:H2' | 1:XA:628:G:C8 | 2.49 | 0.47 |
| 6:XF:27:GLN:O | 6:XF:30:LEU:HG | 2.13 | 0.47 |
| 9:XI:21:PRO:HA | 9:XI:59:PHE:HA | 1.96 | 0.47 |
| 14:YN:4:LYS:HA | 14:YN:7:ILE:HG12 | 1.96 | 0.47 |
| 24:YA:1310:G:OP2 | 52:Y7:9:ARG:NE | 2.34 | 0.47 |
| 24:YA:14:A:H8 | 24:YA:14:A:O5' | 1.97 | 0.47 |
| 24:YA:2070:G:H2' | 24:YA:2071:A:H8 | 1.77 | 0.47 |
| 24:YA:2693:A:H2' | 24:YA:2694:G:H8 | 1.79 | 0.47 |
| 24:YA:662:G:H2' | 24:YA:663:G:H8 | 1.79 | 0.47 |
| 37:YS:34:HIS:ND1 | 37:YS:53:SER:OG | 2.39 | 0.47 |
| 1:QA:1355:G:H2' | 1:QA:1356:G:H8 | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1512:U:H2' | 1:QA:1513:A:C8 | 2.49 | 0.47 |
| 1:QA:181:G:HO2' | 1:QA:182:U:P | 2.36 | 0.47 |
| 1:QA:263:A:OP1 | 20:QT:79:ARG:NH1 | 2.47 | 0.47 |
| 11:QK:62:GLN:HG3 | 11:QK:93:GLN:HB3 | 1.96 | 0.47 |
| 24:RA:2319:G:N1 | 24:RA:2334:G:OP2 | 2.41 | 0.47 |
| 24:RA:37:C:H2' | 24:RA:38:A:C8 | 2.49 | 0.47 |
| 26:RD:148:GLU:HB2 | 26:RD:151:LYS:HD2 | 1.97 | 0.47 |
| 1:XA:509:A:N3 | 1:XA:543:C:O2' | 2.38 | 0.47 |
| 19:XS:32:LYS:HA | 19:XS:50:ALA:HB3 | 1.95 | 0.47 |
| 42:YX:5:TYR:HD2 | 47:Y2:29:LYS:HB2 | 1.79 | 0.47 |
| 50:Y5:49:CYS:O | 50:Y5:56:LYS:HE2 | 2.14 | 0.47 |
| 24:YA:1140:C:OP2 | 32:YN:66:LYS:NZ | 2.42 | 0.47 |
| 24:YA:251:A:C5 | 24:YA:252:G:H1' | 2.49 | 0.47 |
| 24:YA:2698:U:H2' | 24:YA:2699:C:C6 | 2.49 | 0.47 |
| 27:YE:176:ILE:HB | 27:YE:181:LEU:HB2 | 1.96 | 0.47 |
| 27:YE:23:VAL:HG12 | 27:YE:173:VAL:HG21 | 1.95 | 0.47 |
| 34:YP:47:ASP:OD2 | 34:YP:50:ARG:NH2 | 2.47 | 0.47 |
| 1:QA:1009:G:H1 | 1:QA:1020:U:H3 | 1.62 | 0.47 |
| 1:QA:1352:C:H2' | 1:QA:1353:G:C8 | 2.49 | 0.47 |
| 1:QA:244:U:H4' | 1:QA:245:C:O5' | 2.14 | 0.47 |
| 1:QA:437:U:H2' | 1:QA:438:G:O4' | 2.14 | 0.47 |
| 19:QS:64:GLU:OE1 | 49:R4:58:ARG:NH1 | 2.47 | 0.47 |
| 24:RA:1525:G:H2' | 24:RA:1526:G:H8 | 1.80 | 0.47 |
| 24:RA:2832:U:H4' | 24:RA:2833:G:H5'' | 1.97 | 0.47 |
| 24:RA:729:G:OP2 | 26:RD:13:ARG:HD3 | 2.15 | 0.47 |
| 24:RA:729:G:O2' | 24:RA:763:G:H4' | 2.14 | 0.47 |
| 25:RB:111:U:H2' | 25:RB:112:G:H8 | 1.79 | 0.47 |
| 28:RF:116:ASP:OD2 | 34:RP:1:MET:N | 2.34 | 0.47 |
| 1:XA:316:G:OP2 | 1:XA:351:G:O2' | 2.23 | 0.47 |
| 1:XA:407:G:H2' | 1:XA:408:A:C8 | 2.49 | 0.47 |
| 2:XB:235:SER:O | 2:XB:237:ALA:N | 2.45 | 0.47 |
| 5:XE:10:MET:HB3 | 5:XE:32:VAL:HG12 | 1.96 | 0.47 |
| 14:YN:24:CYS:HB2 | 14:YN:27:CYS:SG | 2.54 | 0.47 |
| 24:YA:1882:C:H3' | 24:YA:1883:G:H8 | 1.79 | 0.47 |
| 24:YA:2610:C:H4' | 24:YA:2611:U:OP2 | 2.13 | 0.47 |
| 24:YA:270(V):G:H2' | 24:YA:270(W):G:H8 | 1.80 | 0.47 |
| 24:YA:2728:U:H2' | 24:YA:2729:G:C8 | 2.49 | 0.47 |
| 24:YA:38:A:H2' | 24:YA:39:C:C6 | 2.50 | 0.47 |
| 24:YA:439:G:H2' | 24:YA:440:G:C8 | 2.49 | 0.47 |
| 24:YA:617:G:OP1 | 28:YF:40:GLN:NE2 | 2.47 | 0.47 |
| 24:YA:689:A:H2' | 24:YA:690:G:C8 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:YG:65:GLY:HA3 | 49:Y4:9:LEU:HD21 | 1.95 | 0.47 |
| 24:YA:831:G:O2' | 34:YP:38:GLN:OE1 | 2.32 | 0.47 |
| 44:YZ:45:ASP:OD1 | 44:YZ:49:ARG:NE | 2.47 | 0.47 |
| 1:QA:1034:G:H2' | 1:QA:1035:A:C8 | 2.50 | 0.47 |
| 1:QA:1223:C:P | 1:QA:1224:G:H2' | 2.55 | 0.47 |
| 1:QA:481:G:O2' | 1:QA:482:A:O5' | 2.33 | 0.47 |
| 3:QC:20:SER:OG | 3:QC:22:TRP:NE1 | 2.46 | 0.47 |
| 7:QG:72:ARG:O | 7:QG:91:VAL:HG12 | 2.13 | 0.47 |
| 8:QH:49:GLU:OE2 | 8:QH:62:TYR:OH | 2.27 | 0.47 |
| 11:QK:43:SER:HB3 | 11:QK:68:ALA:HB2 | 1.95 | 0.47 |
| 17:QQ:43:LEU:HD21 | 17:QQ:68:ARG:HH21 | 1.79 | 0.47 |
| 24:RA:1278:A:H2' | 24:RA:1279:G:H8 | 1.78 | 0.47 |
| 24:RA:1309:G:HO2' | 24:RA:1611:C:HO2' | 1.62 | 0.47 |
| 24:RA:121:G:H4' | 24:RA:149:A:H5' | 1.96 | 0.47 |
| 24:RA:1686:C:H3' | 24:RA:1687:G:H8 | 1.79 | 0.47 |
| 24:RA:2522:U:H3 | 24:RA:2543:G:H1 | 1.62 | 0.47 |
| 24:RA:746:A:O2' | 24:RA:2611:U:O2' | 2.30 | 0.47 |
| 24:RA:834:C:H2' | 24:RA:835:A:C8 | 2.48 | 0.47 |
| 28:RF:200:GLU:N | 28:RF:200:GLU:OE2 | 2.43 | 0.47 |
| 29:RG:83:ARG:HD2 | 29:RG:84:LYS:H | 1.79 | 0.47 |
| 1:XA:45:U:H2' | 1:XA:46:G:H8 | 1.80 | 0.47 |
| 1:XA:922:G:H2' | 1:XA:923:A:C8 | 2.50 | 0.47 |
| 4:XD:138:TYR:OH | 4:XD:141:ARG:NH2 | 2.47 | 0.47 |
| 7:XG:75:VAL:HA | 7:XG:88:PRO:HA | 1.96 | 0.47 |
| 13:XM:91:ARG:HH11 | 13:XM:96:LEU:HD22 | 1.79 | 0.47 |
| 52:Y7:13:ALA:HB2 | 52:Y7:46:VAL:HG11 | 1.97 | 0.47 |
| 24:YA:1283:G:N2 | 24:YA:1286:A:OP2 | 2.47 | 0.47 |
| 24:YA:249:C:H5' | 24:YA:2394:C:O2' | 2.15 | 0.47 |
| 24:YA:2692:C:H2' | 24:YA:2693:A:H8 | 1.79 | 0.47 |
| 27:YE:38:THR:OG1 | 27:YE:40:GLU:OE1 | 2.31 | 0.47 |
| 1:QA:398:C:H2' | 1:QA:399:G:H8 | 1.79 | 0.47 |
| 4:QD:127:THR:HA | 4:QD:132:ARG:HA | 1.97 | 0.47 |
| 5:QE:98:THR:HB | 5:QE:117:ASP:HB3 | 1.96 | 0.47 |
| 11:QK:21:ILE:HB | 11:QK:84:VAL:HG23 | 1.96 | 0.47 |
| 12:QL:32:PHE:HD2 | 12:QL:86:ARG:HA | 1.80 | 0.47 |
| 24:RA:1427:A:H4' | 24:RA:1428:C:O5' | 2.14 | 0.47 |
| 24:RA:2246:G:H2' | 24:RA:2247:A:H8 | 1.79 | 0.47 |
| 24:RA:2327:A:H2' | 24:RA:2328:A:C8 | 2.49 | 0.47 |
| 24:RA:593:G:H2' | 24:RA:594:U:C6 | 2.50 | 0.47 |
| 24:RA:639:U:H2' | 24:RA:640:C:C6 | 2.50 | 0.47 |
| 24:RA:678:C:H2' | 24:RA:679:C:C6 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:RA:796:C:H2' | 24:RA:797:C:C6 | 2.49 | 0.47 |
| 28:RF:102:PRO:HB2 | 28:RF:105:VAL:HG23 | 1.96 | 0.47 |
| 28:RF:125:LEU:HA | 28:RF:194:MET:O | 2.15 | 0.47 |
| 32:RN:26:LEU:O | 32:RN:30:ILE:HG13 | 2.14 | 0.47 |
| 1:XA:1287:A:H2 | 1:XA:1353:G:H1' | 1.77 | 0.47 |
| 1:XA:501:C:H2' | 1:XA:502:G:C8 | 2.49 | 0.47 |
| 1:XA:950:U:H2' | 1:XA:951:G:H8 | 1.79 | 0.47 |
| 2:XB:16:HIS:HD2 | 2:XB:210:SER:HA | 1.80 | 0.47 |
| 3:XC:32:LEU:HD13 | 3:XC:59:ARG:HD3 | 1.96 | 0.47 |
| 53:Y8:29:LYS:HG2 | 53:Y8:29:LYS:H | 1.44 | 0.47 |
| 24:YA:2514:U:H2' | 24:YA:2515:C:C6 | 2.50 | 0.47 |
| 24:YA:363(D):G:H2' | 24:YA:363(E):U:C6 | 2.49 | 0.47 |
| 24:YA:949:C:H2' | 24:YA:950:G:C8 | 2.50 | 0.47 |
| 1:QA:171:A:H2' | 1:QA:172:A:C8 | 2.50 | 0.47 |
| 1:QA:323:U:H2' | 1:QA:324:G:O4' | 2.15 | 0.47 |
| 24:RA:489:G:N2 | 24:RA:1321:A:OP1 | 2.48 | 0.47 |
| 24:RA:1509:C:H3' | 24:RA:1510:A:H4' | 1.96 | 0.47 |
| 24:RA:439:G:H2' | 24:RA:440:G:C8 | 2.50 | 0.47 |
| 24:RA:534:U:H2' | 24:RA:535:C:C6 | 2.50 | 0.47 |
| 24:RA:823:G:H2' | 24:RA:824:A:H8 | 1.79 | 0.47 |
| 27:RE:36:ARG:NH1 | 27:RE:85:ASN:OD1 | 2.44 | 0.47 |
| 1:XA:486:U:H2' | 1:XA:487:A:C8 | 2.49 | 0.47 |
| 1:XA:489:C:H2' | 1:XA:490:G:H8 | 1.79 | 0.47 |
| 24:YA:1149:G:H2' | 24:YA:1150:C:C6 | 2.50 | 0.47 |
| 24:YA:1157:G:C2' | 24:YA:1158:C:H5' | 2.45 | 0.47 |
| 24:YA:1427:A:H4' | 24:YA:1428:C:O5' | 2.13 | 0.47 |
| 24:YA:2340:G:H2' | 24:YA:2341:G:H8 | 1.80 | 0.47 |
| 24:YA:2475:C:H42 | 24:YA:2529:G:H22 | 1.62 | 0.47 |
| 24:YA:414:C:H2' | 24:YA:415:A:H8 | 1.80 | 0.47 |
| 24:YA:459:U:H2' | 24:YA:460:A:H8 | 1.79 | 0.47 |
| 24:YA:680:G:H2' | 24:YA:681:G:C8 | 2.49 | 0.47 |
| 24:YA:724:U:H2' | 24:YA:725:G:O4' | 2.14 | 0.47 |
| 31:YI:79:ILE:HB | 31:YI:142:VAL:HA | 1.94 | 0.47 |
| 27:YE:20:ALA:N | 33:YO:72:PRO:O | 2.41 | 0.47 |
| 38:YT:123:GLN:O | 38:YT:125:ARG:N | 2.47 | 0.47 |
| 24:RA:1062:G:H2' | 24:RA:1063:G:C8 | 2.49 | 0.47 |
| 24:RA:13:A:O2' | 24:RA:15:G:N7 | 2.47 | 0.47 |
| 24:RA:2156:G:O6 | 24:RA:2157:G:N2 | 2.43 | 0.47 |
| 24:RA:2749:A:OP2 | 24:RA:2750:A:O2' | 2.24 | 0.47 |
| 24:RA:281:G:H21 | 24:RA:359:A:H62 | 1.61 | 0.47 |
| 1:XA:324:G:H5'' | 20:XT:70:SER:CB | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:XA:377:G:H2' | 1:XA:378:G:C8 | 2.50 | 0.47 |
| 1:XA:452:A:N6 | 1:XA:480:U:C2 | 2.79 | 0.47 |
| 1:XA:685:G:OP1 | 11:XK:11:LYS:NZ | 2.46 | 0.47 |
| 3:XC:70:VAL:HG12 | 3:XC:72:LYS:H | 1.80 | 0.47 |
| 24:YA:1028:A:H2' | 24:YA:1029:A:C8 | 2.49 | 0.47 |
| 31:YI:76:THR:OG1 | 31:YI:139:GLN:NE2 | 2.44 | 0.47 |
| 32:YN:58:ASP:N | 32:YN:58:ASP:OD1 | 2.42 | 0.47 |
| 39:YU:28:ARG:NH1 | 39:YU:38:THR:OG1 | 2.44 | 0.47 |
| 1:QA:426:G:OP1 | 4:QD:38:TYR:OH | 2.25 | 0.47 |
| 1:QA:647:C:H2' | 1:QA:648:A:H8 | 1.79 | 0.47 |
| 13:QM:87:TYR:HB3 | 19:QS:73:GLU:HG3 | 1.97 | 0.47 |
| 46:R1:60:PHE:HE1 | 46:R1:87:PRO:HG3 | 1.80 | 0.47 |
| 24:RA:1114:G:H2' | 24:RA:1115:G:C8 | 2.50 | 0.47 |
| 24:RA:1116:C:H2' | 24:RA:1117:G:H8 | 1.80 | 0.47 |
| 24:RA:2500:U:O2' | 24:RA:2504:U:OP1 | 2.27 | 0.47 |
| 24:RA:2836:U:H2' | 24:RA:2837:G:C8 | 2.49 | 0.47 |
| 24:RA:699:A:H62 | 24:RA:733:G:H21 | 1.62 | 0.47 |
| 24:RA:923:C:H2' | 24:RA:924:C:C6 | 2.50 | 0.47 |
| 36:RR:104:ARG:HE | 36:RR:111:LEU:HD21 | 1.80 | 0.47 |
| 1:XA:891:U:H2' | 1:XA:892:A:H8 | 1.80 | 0.47 |
| 1:XA:438:G:H4' | 4:XD:123:HIS:CG | 2.50 | 0.47 |
| 17:XQ:19:VAL:O | 17:XQ:44:ALA:N | 2.40 | 0.47 |
| 24:YA:1165:U:H2' | 24:YA:1166:C:C6 | 2.49 | 0.47 |
| 24:YA:2040:C:H2' | 24:YA:2041:U:C6 | 2.50 | 0.47 |
| 24:YA:363:G:H2' | 24:YA:363(A):A:H8 | 1.79 | 0.47 |
| 24:YA:924:C:H2' | 24:YA:925:C:C6 | 2.49 | 0.47 |
| 27:YE:50:GLY:HA2 | 27:YE:77:ILE:HA | 1.97 | 0.47 |
| 32:YN:7:LYS:HD3 | 32:YN:8:GLN:H | 1.79 | 0.47 |
| 33:YO:28:SER:OG | 33:YO:29:ASN:N | 2.48 | 0.47 |
| 1:QA:1250:A:H2 | 1:QA:1370:G:H1' | 1.80 | 0.47 |
| 9:QI:32:ASP:HB3 | 9:QI:35:GLU:HG2 | 1.97 | 0.47 |
| 1:QA:707:C:H4' | 11:QK:20:TYR:CD2 | 2.50 | 0.47 |
| 12:QL:32:PHE:CD2 | 12:QL:86:ARG:HA | 2.50 | 0.47 |
| 24:RA:2100:G:H2' | 24:RA:2101:G:C8 | 2.49 | 0.47 |
| 24:RA:2233:U:H2' | 24:RA:2234:G:C8 | 2.50 | 0.47 |
| 24:RA:2051:A:H5' | 24:RA:2578:G:O4' | 2.14 | 0.47 |
| 24:RA:2591:C:H2' | 24:RA:2592:G:C8 | 2.50 | 0.47 |
| 24:RA:2591:C:H2' | 24:RA:2592:G:H8 | 1.79 | 0.47 |
| 24:RA:2857:G:N2 | 24:RA:2860:A:OP2 | 2.38 | 0.47 |
| 24:RA:550:G:H2' | 24:RA:551:G:H8 | 1.80 | 0.47 |
| 1:XA:1463:C:H2' | 1:XA:1464:G:H8 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:596:C:OP2 | 1:XA:597:G:OP2 | 2.32 | 0.47 |
| 24:YA:2099:U:O2 | 24:YA:2190:G:N2 | 2.40 | 0.47 |
| 24:YA:2115:G:N2 | 24:YA:2164:C:OP2 | 2.47 | 0.47 |
| 24:YA:2061:G:H5'' | 24:YA:2503:A:C2 | 2.50 | 0.47 |
| 24:YA:264:C:C2' | 24:YA:265:A:H5'' | 2.44 | 0.47 |
| 24:YA:271(D):G:H2' | 24:YA:272:G:C8 | 2.50 | 0.47 |
| 24:YA:358:U:H2' | 24:YA:359:A:C8 | 2.49 | 0.47 |
| 26:YD:16:MET:HG3 | 26:YD:207:GLY:HA3 | 1.97 | 0.47 |
| 1:QA:1043:C:H2' | 1:QA:1044:A:C8 | 2.50 | 0.47 |
| 1:QA:1238:A:H62 | 1:QA:1301:U:H3 | 1.62 | 0.47 |
| 1:QA:1371:G:OP1 | 9:QI:11:LYS:NZ | 2.41 | 0.47 |
| 6:QF:47:ARG:NH2 | 6:QF:56:PRO:O | 2.48 | 0.47 |
| 10:QJ:41:PRO:HG2 | 10:QJ:43:ARG:HH12 | 1.80 | 0.47 |
| 47:R2:9:GLN:HE22 | 47:R2:60:LEU:HD21 | 1.78 | 0.47 |
| 24:RA:186:G:H2' | 24:RA:187:G:H8 | 1.79 | 0.47 |
| 24:RA:2130:U:H2' | 24:RA:2131:G:C8 | 2.49 | 0.47 |
| 24:RA:29:U:H2' | 24:RA:30:G:C8 | 2.48 | 0.47 |
| 24:RA:634:C:H2' | 24:RA:635:C:C6 | 2.49 | 0.47 |
| 24:RA:907:U:O2' | 35:RQ:101:ARG:NH2 | 2.45 | 0.47 |
| 38:RT:124:ASP:N | 38:RT:124:ASP:OD2 | 2.48 | 0.47 |
| 1:XA:1253:G:H4' | 10:XJ:46:ARG:NH1 | 2.29 | 0.47 |
| 1:XA:677:U:O2 | 1:XA:777:A:O2' | 2.33 | 0.47 |
| 1:XA:762:C:H2' | 1:XA:763:G:H8 | 1.78 | 0.47 |
| 2:XB:145:LEU:HD13 | 2:XB:145:LEU:HA | 1.54 | 0.47 |
| 24:YA:1826:G:OP1 | 26:YD:224:ALA:N | 2.46 | 0.47 |
| 24:YA:2502:G:H5'' | 24:YA:2503:A:H5'' | 1.97 | 0.47 |
| 24:YA:2804:C:H2' | 24:YA:2805:G:C8 | 2.50 | 0.47 |
| 24:YA:2853:C:H2' | 24:YA:2854:G:C8 | 2.49 | 0.47 |
| 24:YA:532:A:H4' | 24:YA:533:G:C8 | 2.50 | 0.47 |
| 36:YR:38:VAL:HG12 | 36:YR:112:ALA:HB2 | 1.97 | 0.47 |
| 40:YV:23:GLU:OE2 | 40:YV:89:GLN:NE2 | 2.40 | 0.47 |
| 40:YV:52:VAL:O | 40:YV:53:GLU:HG2 | 2.15 | 0.47 |
| 1:QA:1066:C:H3' | 1:QA:1067:A:C8 | 2.50 | 0.47 |
| 1:QA:1329:A:N7 | 21:QU:7:ARG:NH2 | 2.61 | 0.47 |
| 13:QM:16:ASP:N | 13:QM:16:ASP:OD1 | 2.47 | 0.47 |
| 24:RA:1167:U:H2' | 24:RA:1168:G:H8 | 1.79 | 0.47 |
| 24:RA:576:U:OP1 | 24:RA:2503:A:OP1 | 2.32 | 0.47 |
| 25:RB:77:U:P | 44:RZ:19:ARG:HH22 | 2.38 | 0.47 |
| 26:RD:158:ALA:O | 26:RD:196:VAL:HG21 | 2.15 | 0.47 |
| 24:RA:674:G:H1' | 28:RF:74:ARG:HD3 | 1.97 | 0.47 |
| 37:RS:83:LYS:HE2 | 37:RS:109:GLY:HA3 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:287:U:H2' | 1:XA:288:A:H8 | 1.80 | 0.47 |
| 1:XA:552:U:H2' | 1:XA:553:A:C8 | 2.50 | 0.47 |
| 1:XA:745:C:OP1 | 1:XA:851:G:O2' | 2.33 | 0.47 |
| 5:XE:135:THR:O | 5:XE:139:LEU:HG | 2.15 | 0.47 |
| 45:Y0:27:GLU:HG3 | 45:Y0:68:GLU:HA | 1.96 | 0.47 |
| 24:YA:2306:C:H2' | 24:YA:2307:G:N2 | 2.30 | 0.47 |
| 24:YA:270(R):G:H2' | 24:YA:270(S):G:H8 | 1.80 | 0.47 |
| 24:YA:2808:U:C2 | 24:YA:2892:A:N6 | 2.83 | 0.47 |
| 24:YA:305:U:H2' | 24:YA:306:U:C6 | 2.50 | 0.47 |
| 24:YA:441:U:H2' | 24:YA:442:G:C8 | 2.50 | 0.47 |
| 24:YA:634:C:H2' | 24:YA:635:C:C6 | 2.50 | 0.47 |
| 24:YA:2749:A:OP1 | 30:YH:4:ILE:HG23 | 2.15 | 0.47 |
| 1:QA:318:G:H2' | 1:QA:319:G:H8 | 1.79 | 0.46 |
| 1:QA:782:A:H62 | 1:QA:800:G:N2 | 2.10 | 0.46 |
| 1:QA:790:A:H2' | 1:QA:791:G:C8 | 2.49 | 0.46 |
| 3:QC:62:ASP:O | 3:QC:97:LYS:HB3 | 2.15 | 0.46 |
| 4:QD:64:LEU:HD12 | 4:QD:198:VAL:HG11 | 1.97 | 0.46 |
| 13:QM:49:THR:HG22 | 13:QM:51:ALA:H | 1.80 | 0.46 |
| 1:QA:1325:C:H4' | 21:QU:17:THR:HG21 | 1.97 | 0.46 |
| 24:RA:1050:A:H2' | 24:RA:1051:G:O4' | 2.15 | 0.46 |
| 24:RA:1141:U:H1' | 24:RA:1142(A):A:C6 | 2.50 | 0.46 |
| 24:RA:1666:G:N3 | 33:RO:3:GLN:NE2 | 2.63 | 0.46 |
| 24:RA:2025:C:H2' | 24:RA:2026:C:C6 | 2.49 | 0.46 |
| 24:RA:2102:U:H2' | 24:RA:2103:C:C6 | 2.50 | 0.46 |
| 24:RA:2291:U:O2' | 24:RA:2374:C:O2 | 2.33 | 0.46 |
| 24:RA:575:A:OP2 | 24:RA:2499:C:O2' | 2.27 | 0.46 |
| 24:RA:822:U:H2' | 24:RA:823:G:C8 | 2.50 | 0.46 |
| 26:RD:247:ALA:HA | 26:RD:253:GLN:HA | 1.96 | 0.46 |
| 43:RY:77:PRO:HD3 | 43:RY:106:LEU:HD13 | 1.97 | 0.46 |
| 24:RA:84:A:OP2 | 43:RY:97:ARG:NH2 | 2.48 | 0.46 |
| 1:XA:1279:A:O2' | 1:XA:1282:C:N4 | 2.49 | 0.46 |
| 2:XB:12:GLU:OE2 | 2:XB:12:GLU:N | 2.48 | 0.46 |
| 4:XD:105:VAL:HG23 | 4:XD:117:ALA:HB1 | 1.97 | 0.46 |
| 6:XF:25:ILE:O | 6:XF:28:ARG:HG3 | 2.15 | 0.46 |
| 29:YG:109:VAL:HG13 | 49:Y4:33:VAL:HG21 | 1.98 | 0.46 |
| 24:YA:86:C:H4' | 24:YA:104:U:H1' | 1.97 | 0.46 |
| 24:YA:1136:G:H2' | 24:YA:1137:G:C8 | 2.50 | 0.46 |
| 24:YA:1824:G:N3 | 26:YD:254:THR:OG1 | 2.47 | 0.46 |
| 25:YB:31:C:O2' | 25:YB:53:A:N1 | 2.43 | 0.46 |
| 1:QA:1111:A:N1 | 3:QC:177:THR:HG22 | 2.31 | 0.46 |
| 1:QA:737:A:H2' | 1:QA:738:C:C6 | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:QL:46:LYS:HG3 | 12:QL:48:PRO:HD3 | 1.97 | 0.46 |
| 24:RA:1539:G:H2' | 24:RA:1540:G:H8 | 1.81 | 0.46 |
| 24:RA:2245:U:C5' | 24:RA:2246:G:H5' | 2.42 | 0.46 |
| 24:RA:2461:C:H2' | 24:RA:2462:U:C6 | 2.50 | 0.46 |
| 24:RA:2471:C:H3' | 24:RA:2472:G:H8 | 1.80 | 0.46 |
| 24:RA:2023:G:H5' | 24:RA:2617:C:H4' | 1.97 | 0.46 |
| 24:RA:2870:C:H2' | 24:RA:2871:C:O4' | 2.15 | 0.46 |
| 24:RA:44:A:H2' | 24:RA:45:G:C8 | 2.50 | 0.46 |
| 1:XA:280:C:H3' | 1:XA:281:G:H5' | 1.97 | 0.46 |
| 1:XA:851:G:H2' | 1:XA:852:G:C8 | 2.50 | 0.46 |
| 13:XM:13:LYS:HB3 | 13:XM:44:ARG:HH21 | 1.80 | 0.46 |
| 24:YA:1055:G:O2' | 24:YA:1085:A:N1 | 2.39 | 0.46 |
| 24:YA:2443:C:H2' | 24:YA:2444:G:H8 | 1.79 | 0.46 |
| 24:YA:2816:C:H2' | 24:YA:2817:G:H8 | 1.80 | 0.46 |
| 24:YA:363(B):G:H2' | 24:YA:363(C):G:C8 | 2.51 | 0.46 |
| 1:QA:664:G:H22 | 1:QA:741:G:H1 | 1.62 | 0.46 |
| 24:RA:2361:A:O5' | 53:R8:27:THR:OG1 | 2.33 | 0.46 |
| 24:RA:1084:A:H5'' | 24:RA:1085:A:C8 | 2.50 | 0.46 |
| 24:RA:226:G:H2' | 24:RA:227:A:C8 | 2.51 | 0.46 |
| 24:RA:232:G:H8 | 24:RA:232:G:OP2 | 1.99 | 0.46 |
| 33:RO:98:VAL:HG12 | 33:RO:117:LEU:HB3 | 1.97 | 0.46 |
| 1:XA:1151:A:H2' | 1:XA:1152:A:H8 | 1.79 | 0.46 |
| 1:XA:1435:G:H2' | 1:XA:1436:U:C6 | 2.50 | 0.46 |
| 1:XA:188:U:H2' | 1:XA:189:U:H5'' | 1.98 | 0.46 |
| 1:XA:92:G:H2' | 1:XA:93:U:C2 | 2.50 | 0.46 |
| 2:XB:84:GLU:HB3 | 2:XB:219:VAL:HG21 | 1.97 | 0.46 |
| 5:XE:105:VAL:HG13 | 5:XE:106:PRO:HD3 | 1.96 | 0.46 |
| 5:XE:137:GLU:OE1 | 5:XE:140:ARG:NH1 | 2.48 | 0.46 |
| 10:XJ:79:ARG:HE | 10:XJ:82:ILE:HD12 | 1.80 | 0.46 |
| 11:XK:17:GLY:HA2 | 11:XK:35:PRO:HD3 | 1.97 | 0.46 |
| 24:YA:2199:A:OP1 | 46:Y1:50:ARG:NH2 | 2.48 | 0.46 |
| 24:YA:857:C:OP1 | 45:Y0:69:PHE:HD2 | 1.99 | 0.46 |
| 26:YD:44:ASN:HB3 | 26:YD:49:ILE:HA | 1.97 | 0.46 |
| 28:YF:77:ASP:OD1 | 28:YF:77:ASP:N | 2.46 | 0.46 |
| 1:QA:711:G:H2' | 1:QA:712:A:H8 | 1.79 | 0.46 |
| 24:RA:1657:C:O3' | 27:RE:133:LYS:CG | 2.48 | 0.46 |
| 24:RA:2572:A:H2' | 27:RE:144:ARG:HD3 | 1.97 | 0.46 |
| 24:RA:2693:A:H2' | 24:RA:2694:G:H8 | 1.80 | 0.46 |
| 24:RA:414:C:H2' | 24:RA:415:A:C8 | 2.50 | 0.46 |
| 24:RA:65:C:H2' | 24:RA:66:C:H6 | 1.80 | 0.46 |
| 26:RD:72:LYS:HG3 | 26:RD:97:TYR:CE2 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:RG:31:VAL:O | 29:RG:33:ARG:NH1 | 2.40 | 0.46 |
| 24:RA:1654:A:P | 36:RR:2:ARG:HG2 | 2.56 | 0.46 |
| 1:XA:22:G:H2' | 1:XA:23:C:C6 | 2.51 | 0.46 |
| 1:XA:753:A:H4' | 1:XA:754:C:O5' | 2.14 | 0.46 |
| 24:YA:2612:C:OP2 | 50:Y5:2:ALA:N | 2.48 | 0.46 |
| 24:YA:1353:A:H2' | 24:YA:1354:A:C8 | 2.50 | 0.46 |
| 24:YA:767:U:H2' | 24:YA:768:G:H8 | 1.81 | 0.46 |
| 27:YE:49:LEU:HD12 | 27:YE:49:LEU:HA | 1.71 | 0.46 |
| 36:YR:56:LYS:HE3 | 36:YR:88:ARG:HA | 1.98 | 0.46 |
| 40:YV:38:LEU:HD11 | 40:YV:57:VAL:HG12 | 1.97 | 0.46 |
| 1:QA:328:C:H4' | 1:QA:329:A:H5' | 1.97 | 0.46 |
| 1:QA:703:G:H4' | 1:QA:704:A:O5' | 2.14 | 0.46 |
| 2:QB:178:ARG:HA | 2:QB:178:ARG:HD3 | 1.69 | 0.46 |
| 13:QM:92:HIS:CE1 | 13:QM:98:VAL:HG21 | 2.50 | 0.46 |
| 1:QA:735:C:H5' | 18:QR:71:LYS:HE3 | 1.98 | 0.46 |
| 24:RA:511:U:H4' | 24:RA:1235:G:H4' | 1.97 | 0.46 |
| 24:RA:1539:G:H2' | 24:RA:1540:G:C8 | 2.51 | 0.46 |
| 24:RA:2246:G:H2' | 24:RA:2247:A:C8 | 2.51 | 0.46 |
| 24:RA:526:A:OP1 | 24:RA:527:C:OP1 | 2.33 | 0.46 |
| 24:RA:638:G:H2' | 24:RA:639:U:C6 | 2.50 | 0.46 |
| 40:RV:38:LEU:HD21 | 40:RV:57:VAL:HG13 | 1.96 | 0.46 |
| 1:XA:1101:A:N6 | 2:XB:176:GLU:OE2 | 2.48 | 0.46 |
| 1:XA:712:A:H2' | 1:XA:713:G:C8 | 2.50 | 0.46 |
| 8:XH:9:MET:O | 8:XH:13:ILE:HG12 | 2.15 | 0.46 |
| 24:YA:1012:U:H2' | 24:YA:1013:C:OP2 | 2.14 | 0.46 |
| 24:YA:2461:C:H2' | 24:YA:2462:U:C6 | 2.50 | 0.46 |
| 24:YA:809:G:H2' | 24:YA:810:U:C6 | 2.50 | 0.46 |
| 40:YV:24:LYS:HA | 40:YV:92:THR:HG23 | 1.96 | 0.46 |
| 1:QA:1014:A:H2' | 1:QA:1015:A:C8 | 2.50 | 0.46 |
| 1:QA:1287:A:H2' | 1:QA:1288:A:H8 | 1.80 | 0.46 |
| 1:QA:973:G:H3' | 1:QA:974:A:H5'' | 1.96 | 0.46 |
| 3:QC:59:ARG:NH1 | 3:QC:62:ASP:H | 2.12 | 0.46 |
| 10:QJ:13:HIS:HA | 10:QJ:16:LEU:HB2 | 1.98 | 0.46 |
| 45:R0:18:ALA:O | 45:R0:20:ARG:NH1 | 2.44 | 0.46 |
| 24:RA:1297:C:H2' | 24:RA:1298:C:H6 | 1.81 | 0.46 |
| 24:RA:2086:U:H2' | 24:RA:2087:G:C8 | 2.51 | 0.46 |
| 24:RA:2341:G:H2' | 24:RA:2342:C:C6 | 2.50 | 0.46 |
| 24:RA:23:G:OP1 | 24:RA:504:U:N3 | 2.40 | 0.46 |
| 24:RA:380:U:H2' | 24:RA:381:G:C8 | 2.50 | 0.46 |
| 24:RA:514:A:H2' | 24:RA:515:A:C8 | 2.51 | 0.46 |
| 1:XA:1055:A:H62 | 1:XA:1200:C:H42 | 1.63 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:79:G:H2' | 1:XA:80:G:C8 | 2.50 | 0.46 |
| 11:XK:86:GLY:N | 11:XK:112:THR:OG1 | 2.46 | 0.46 |
| 1:XA:755:G:OP2 | 15:XO:65:ARG:HD2 | 2.15 | 0.46 |
| 22:XV:54:G:O2' | 22:XV:55:U:O5' | 2.30 | 0.46 |
| 51:Y6:11:LEU:HB2 | 51:Y6:21:TYR:HB2 | 1.98 | 0.46 |
| 24:YA:1333:C:H2' | 24:YA:1334:G:H8 | 1.81 | 0.46 |
| 24:YA:195:A:H5'' | 24:YA:196:A:O5' | 2.16 | 0.46 |
| 29:YG:81:LYS:O | 29:YG:82:LEU:HB2 | 2.15 | 0.46 |
| 1:QA:1479:C:H2' | 1:QA:1480:G:C8 | 2.51 | 0.46 |
| 1:QA:348:G:H2' | 1:QA:349:A:H8 | 1.80 | 0.46 |
| 1:QA:539:A:H2' | 1:QA:540:G:H8 | 1.81 | 0.46 |
| 2:QB:73:THR:O | 2:QB:78:GLN:NE2 | 2.44 | 0.46 |
| 47:R2:18:PRO:HA | 47:R2:21:LEU:HB2 | 1.98 | 0.46 |
| 49:R4:40:HIS:CE1 | 49:R4:42:PHE:HB3 | 2.50 | 0.46 |
| 24:RA:1173:G:N2 | 24:RA:1175:U:O4 | 2.47 | 0.46 |
| 24:RA:1590:U:H2' | 24:RA:1591:G:H8 | 1.80 | 0.46 |
| 31:RI:74:ASN:OD1 | 31:RI:74:ASN:N | 2.47 | 0.46 |
| 1:XA:312:C:H2' | 1:XA:313:A:C8 | 2.51 | 0.46 |
| 1:XA:36:C:H2' | 1:XA:37:U:O4' | 2.15 | 0.46 |
| 1:XA:464:G:C6 | 1:XA:466:C:H5' | 2.50 | 0.46 |
| 2:XB:192:SER:OG | 2:XB:193:ASP:N | 2.49 | 0.46 |
| 12:XL:89:ARG:HD2 | 12:XL:97:ARG:HA | 1.97 | 0.46 |
| 15:XO:7:GLU:HA | 15:XO:10:LYS:HD3 | 1.98 | 0.46 |
| 47:Y2:28:LYS:HD2 | 47:Y2:53:LEU:HD11 | 1.98 | 0.46 |
| 24:YA:1499:C:H2' | 24:YA:1500:G:H8 | 1.81 | 0.46 |
| 24:YA:2086:U:H2' | 24:YA:2087:G:C8 | 2.50 | 0.46 |
| 28:YF:32:LEU:HD11 | 28:YF:105:VAL:HG13 | 1.97 | 0.46 |
| 1:QA:224:C:H2' | 1:QA:225:C:C6 | 2.51 | 0.46 |
| 24:RA:1819:A:H4' | 24:RA:1820:U:O5' | 2.16 | 0.46 |
| 24:RA:1326:U:HO2' | 24:RA:2010:G:HO2' | 1.63 | 0.46 |
| 24:RA:2365:G:OP1 | 45:R0:55:ARG:HD2 | 2.16 | 0.46 |
| 24:RA:2630:G:H2' | 24:RA:2631:G:C8 | 2.50 | 0.46 |
| 39:RU:90:VAL:HG13 | 40:RV:39:LEU:HD22 | 1.97 | 0.46 |
| 24:RA:64:A:O3' | 42:RX:71:GLY:HA3 | 2.16 | 0.46 |
| 1:XA:173:U:H5'' | 1:XA:197:A:O4' | 2.15 | 0.46 |
| 1:XA:359:U:H5 | 1:XA:359:U:OP2 | 1.99 | 0.46 |
| 1:XA:711:G:H2' | 1:XA:712:A:C8 | 2.51 | 0.46 |
| 20:XT:53:LEU:HD21 | 20:XT:100:ILE:HB | 1.98 | 0.46 |
| 24:YA:1220:A:H5' | 24:YA:1221:C:OP2 | 2.16 | 0.46 |
| 24:YA:1332:G:N2 | 24:YA:1610:A:N7 | 2.56 | 0.46 |
| 24:YA:2476:A:H2' | 24:YA:2477:C:C6 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:YA:834:C:H2' | 24:YA:835:A:H8 | 1.80 | 0.46 |
| 24:YA:2618:G:H21 | 27:YE:150:VAL:HG21 | 1.80 | 0.46 |
| 29:YG:15:VAL:HG13 | 29:YG:175:LEU:HB2 | 1.98 | 0.46 |
| 24:YA:2406:U:C2 | 34:YP:72:PRO:HB2 | 2.51 | 0.46 |
| 1:QA:1285:A:H1' | 1:QA:1286:A:OP2 | 2.16 | 0.46 |
| 1:QA:1391:U:H2' | 1:QA:1392:G:C8 | 2.51 | 0.46 |
| 22:QV:2:G:H2' | 22:QV:3:G:C8 | 2.51 | 0.46 |
| 24:RA:1045:A:O4' | 24:RA:1111:A:N6 | 2.49 | 0.46 |
| 24:RA:2788:C:O2' | 24:RA:2809:A:N3 | 2.47 | 0.46 |
| 24:RA:84:A:N1 | 24:RA:98:G:O2' | 2.38 | 0.46 |
| 28:RF:124:LEU:HB3 | 28:RF:193:VAL:HG23 | 1.98 | 0.46 |
| 29:RG:24:GLY:O | 29:RG:26:GLN:NE2 | 2.49 | 0.46 |
| 31:RI:116:LEU:HD21 | 31:RI:119:PRO:HA | 1.98 | 0.46 |
| 1:XA:1100:C:H3' | 2:XB:96:ARG:HH21 | 1.81 | 0.46 |
| 1:XA:1244:C:H2' | 1:XA:1245:A:C8 | 2.51 | 0.46 |
| 1:XA:1355:G:H2' | 1:XA:1356:G:C8 | 2.50 | 0.46 |
| 1:XA:1233:G:O2' | 1:XA:1365:G:OP1 | 2.32 | 0.46 |
| 1:XA:1440:C:H2' | 1:XA:1441:G:O4' | 2.16 | 0.46 |
| 1:XA:244:U:H4' | 1:XA:245:C:C5' | 2.46 | 0.46 |
| 45:Y0:38:VAL:HB | 45:Y0:59:LEU:HB2 | 1.98 | 0.46 |
| 24:YA:1191:G:OP1 | 34:YP:18:ARG:NH2 | 2.49 | 0.46 |
| 24:YA:1825:A:H4' | 26:YD:233:HIS:HE1 | 1.81 | 0.46 |
| 24:YA:270(J):G:H1 | 24:YA:270(P):C:H42 | 1.62 | 0.46 |
| 24:YA:363(C):G:H2' | 24:YA:363(D):G:H8 | 1.81 | 0.46 |
| 24:YA:729:G:P | 26:YD:13:ARG:HD3 | 2.55 | 0.46 |
| 35:YQ:58:PHE:HD2 | 35:YQ:61:GLY:HA3 | 1.80 | 0.46 |
| 1:QA:106:C:H2' | 1:QA:107:G:H8 | 1.80 | 0.46 |
| 1:QA:475:G:H2' | 1:QA:476:G:H8 | 1.80 | 0.46 |
| 1:QA:638:G:H2' | 1:QA:639:G:H8 | 1.80 | 0.46 |
| 9:QI:10:ARG:O | 9:QI:13:ALA:HB3 | 2.17 | 0.46 |
| 12:QL:103:GLY:N | 12:QL:107:ALA:O | 2.50 | 0.46 |
| 14:QN:29:ARG:HH22 | 14:QN:42:ILE:H | 1.63 | 0.46 |
| 24:RA:2625:G:H2' | 24:RA:2626:C:C6 | 2.51 | 0.46 |
| 24:RA:639:U:H2' | 24:RA:640:C:H6 | 1.81 | 0.46 |
| 24:RA:971:C:H2' | 24:RA:972:G:O4' | 2.16 | 0.46 |
| 27:RE:36:ARG:HG3 | 27:RE:47:VAL:HG12 | 1.98 | 0.46 |
| 1:XA:119:A:H4' | 1:XA:120:A:C8 | 2.51 | 0.46 |
| 1:XA:1323:G:H2' | 1:XA:1324:A:C8 | 2.51 | 0.46 |
| 1:XA:1512:U:H2' | 1:XA:1513:A:H8 | 1.81 | 0.46 |
| 1:XA:556:C:H2' | 1:XA:557:G:H8 | 1.81 | 0.46 |
| 5:XE:78:HIS:HB2 | 8:XH:104:ARG:HB3 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:Y1:18:ILE:HG12 | 46:Y1:37:ILE:HG12 | 1.98 | 0.46 |
| 49:Y4:16:CYS:HB3 | 49:Y4:20:ASN:HB3 | 1.97 | 0.46 |
| 24:YA:1359:A:N6 | 24:YA:1372:U:N3 | 2.37 | 0.46 |
| 24:YA:570:G:H2' | 24:YA:2030:A:C5 | 2.51 | 0.46 |
| 24:YA:2572:A:H2' | 27:YE:144:ARG:HD3 | 1.98 | 0.46 |
| 24:YA:597:U:H2' | 24:YA:598:G:H8 | 1.80 | 0.46 |
| 36:YR:79:LEU:HD12 | 36:YR:83:ILE:HB | 1.98 | 0.46 |
| 24:RA:1435:G:H2' | 24:RA:1436:G:C8 | 2.51 | 0.45 |
| 24:RA:223:A:O2' | 24:RA:420:C:O2 | 2.34 | 0.45 |
| 30:RH:137:ASP:HB3 | 30:RH:140:LYS:HB3 | 1.98 | 0.45 |
| 30:RH:91:GLY:HA3 | 30:RH:94:TYR:CD2 | 2.51 | 0.45 |
| 1:XA:1203:C:H2' | 1:XA:1204:A:H8 | 1.81 | 0.45 |
| 1:XA:1240:U:OP1 | 7:XG:119:ARG:NH2 | 2.49 | 0.45 |
| 1:XA:997:U:H2' | 1:XA:998:G:H8 | 1.79 | 0.45 |
| 8:XH:41:ARG:NH2 | 8:XH:123:GLU:OE2 | 2.48 | 0.45 |
| 22:XV:24:C:H2' | 22:XV:25:G:C8 | 2.51 | 0.45 |
| 24:YA:126:A:H61 | 52:Y7:42:LEU:HD12 | 1.81 | 0.45 |
| 24:YA:1178:C:H2' | 24:YA:1179:C:C6 | 2.51 | 0.45 |
| 24:YA:963:U:H1' | 24:YA:2250:G:O6 | 2.16 | 0.45 |
| 24:YA:619:G:H3' | 24:YA:620:G:H21 | 1.80 | 0.45 |
| 27:YE:45:THR:O | 27:YE:83:ASP:N | 2.46 | 0.45 |
| 35:YQ:48:GLU:OE2 | 35:YQ:51:ARG:NH2 | 2.36 | 0.45 |
| 41:YW:69:LEU:HD23 | 41:YW:107:LEU:HD13 | 1.97 | 0.45 |
| 44:YZ:52:SER:OG | 44:YZ:52:SER:O | 2.29 | 0.45 |
| 1:QA:10:A:H2' | 1:QA:11:G:H8 | 1.82 | 0.45 |
| 1:QA:1118:C:H1' | 1:QA:1179:A:C4 | 2.50 | 0.45 |
| 1:QA:397:A:N7 | 1:QA:547:A:O2' | 2.48 | 0.45 |
| 1:QA:711:G:OP2 | 6:QF:54:LYS:NZ | 2.48 | 0.45 |
| 1:QA:921:U:O2' | 5:QE:19:MET:O | 2.29 | 0.45 |
| 11:QK:91:ARG:O | 11:QK:95:ILE:HG13 | 2.16 | 0.45 |
| 53:R8:54:GLU:O | 53:R8:58:ILE:HG13 | 2.16 | 0.45 |
| 24:RA:1246:A:OP1 | 34:RP:15:ARG:NH2 | 2.44 | 0.45 |
| 24:RA:1519:G:H3' | 24:RA:1520:U:H6 | 1.80 | 0.45 |
| 24:RA:1676:A:C2 | 24:RA:1993:U:H5' | 2.52 | 0.45 |
| 24:RA:1791:A:H4' | 26:RD:206:LEU:HB2 | 1.98 | 0.45 |
| 24:RA:1990:C:H2' | 24:RA:1991:U:C6 | 2.51 | 0.45 |
| 24:RA:570:G:H2' | 24:RA:2030:A:C5 | 2.51 | 0.45 |
| 24:RA:840:C:H2' | 24:RA:841:A:C8 | 2.51 | 0.45 |
| 25:RB:37:C:O2 | 37:RS:95:HIS:NE2 | 2.49 | 0.45 |
| 40:RV:4:ILE:HG22 | 40:RV:39:LEU:HD13 | 1.97 | 0.45 |
| 1:XA:1189:C:H5'' | 3:XC:5:ILE:HG21 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:XA:1228:C:OP1 | 13:XM:115:LYS:HG2 | 2.16 | 0.45 |
| 1:XA:164:U:H2' | 1:XA:165:C:C6 | 2.51 | 0.45 |
| 4:XD:104:VAL:O | 4:XD:108:LEU:HG | 2.16 | 0.45 |
| 9:XI:111:ARG:HH12 | 9:XI:113:LYS:HA | 1.81 | 0.45 |
| 24:YA:1580:A:H5'' | 24:YA:1581:G:C8 | 2.51 | 0.45 |
| 24:YA:2124:G:H3' | 24:YA:2125:G:C8 | 2.50 | 0.45 |
| 24:YA:593:G:H2' | 24:YA:594:U:C6 | 2.51 | 0.45 |
| 24:YA:855:G:H1 | 24:YA:922:U:H3 | 1.64 | 0.45 |
| 1:QA:1400:C:O4' | 23:QX:21:G:O6 | 2.34 | 0.45 |
| 1:QA:382:A:H2' | 1:QA:383:A:C8 | 2.52 | 0.45 |
| 1:QA:477:G:H2' | 1:QA:478:A:H8 | 1.80 | 0.45 |
| 1:QA:486:U:H2' | 1:QA:487:A:C8 | 2.52 | 0.45 |
| 1:QA:22:G:OP1 | 1:QA:561:U:H1' | 2.16 | 0.45 |
| 7:QG:100:ALA:O | 7:QG:104:LEU:HG | 2.15 | 0.45 |
| 10:QJ:92:THR:OG1 | 10:QJ:93:GLY:N | 2.48 | 0.45 |
| 24:RA:1464:C:O2' | 24:RA:1528:A:H8 | 1.99 | 0.45 |
| 24:RA:222:A:H62 | 24:RA:232:G:N2 | 2.14 | 0.45 |
| 24:RA:2567:G:H2' | 24:RA:2568:C:C6 | 2.51 | 0.45 |
| 24:RA:558:G:OP1 | 32:RN:112:LEU:N | 2.50 | 0.45 |
| 25:RB:16:G:H2' | 25:RB:17:C:H6 | 1.82 | 0.45 |
| 35:RQ:4:PRO:HG3 | 35:RQ:69:PHE:HE2 | 1.82 | 0.45 |
| 1:XA:139:G:H2' | 1:XA:140:A:H8 | 1.80 | 0.45 |
| 1:XA:738:C:OP1 | 6:XF:2:ARG:NH1 | 2.46 | 0.45 |
| 1:XA:885:G:H2' | 1:XA:886:G:H8 | 1.81 | 0.45 |
| 4:XD:20:TYR:CD1 | 4:XD:106:TYR:OH | 2.65 | 0.45 |
| 18:XR:32:ARG:HA | 18:XR:69:THR:HG21 | 1.98 | 0.45 |
| 24:YA:1678:G:H2' | 24:YA:1679:U:H6 | 1.82 | 0.45 |
| 24:YA:242:G:H1' | 24:YA:243:U:OP2 | 2.17 | 0.45 |
| 24:YA:304:G:H2' | 24:YA:305:U:C6 | 2.51 | 0.45 |
| 24:YA:755:C:H2' | 24:YA:756:C:C6 | 2.51 | 0.45 |
| 24:YA:760:G:H2' | 24:YA:761:A:O4' | 2.16 | 0.45 |
| 1:QA:1172:C:H2' | 1:QA:1173:G:C8 | 2.50 | 0.45 |
| 1:QA:1298:C:H4' | 1:QA:1299:A:C4 | 2.52 | 0.45 |
| 1:QA:711:G:H2' | 1:QA:712:A:C8 | 2.52 | 0.45 |
| 9:QI:47:LEU:HB2 | 9:QI:50:LEU:HD12 | 1.99 | 0.45 |
| 52:R7:13:ALA:HB2 | 52:R7:46:VAL:HG21 | 1.99 | 0.45 |
| 24:RA:1490:A:O2' | 26:RD:99:ASP:OD1 | 2.34 | 0.45 |
| 24:RA:1825:A:H2' | 24:RA:1826:G:C8 | 2.51 | 0.45 |
| 24:RA:250:G:H2' | 24:RA:251:A:C8 | 2.51 | 0.45 |
| 24:RA:83:G:H1 | 24:RA:102:G:HO2' | 1.61 | 0.45 |
| 28:RF:158:THR:HG23 | 28:RF:160:ASN:H | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:1167:A:H2' | 1:XA:1169:A:C8 | 2.52 | 0.45 |
| 1:XA:1313:U:H2' | 1:XA:1314:C:C6 | 2.51 | 0.45 |
| 1:XA:1425:U:H3 | 1:XA:1475:G:H1 | 1.64 | 0.45 |
| 1:XA:115:G:C6 | 1:XA:313:A:C6 | 3.04 | 0.45 |
| 1:XA:444:C:H2' | 1:XA:445:G:C8 | 2.52 | 0.45 |
| 3:XC:134:ILE:O | 3:XC:138:VAL:HG23 | 2.16 | 0.45 |
| 22:XV:36:G:H2' | 22:XV:37:G:H8 | 1.81 | 0.45 |
| 24:YA:1652:A:OP1 | 36:YR:8:ARG:NH1 | 2.45 | 0.45 |
| 24:YA:2845:G:H2' | 24:YA:2846:G:C8 | 2.52 | 0.45 |
| 24:YA:503:A:H4' | 24:YA:504:U:C5' | 2.46 | 0.45 |
| 24:YA:820:A:H2' | 24:YA:821:A:C8 | 2.52 | 0.45 |
| 24:YA:1490:A:O2' | 26:YD:99:ASP:OD1 | 2.35 | 0.45 |
| 37:YS:78:LEU:HD11 | 37:YS:108:GLY:HA3 | 1.98 | 0.45 |
| 37:YS:109:GLY:O | 37:YS:110:LEU:HG | 2.17 | 0.45 |
| 1:QA:1022:G:H2' | 1:QA:1023:G:C8 | 2.51 | 0.45 |
| 1:QA:1060:C:H2' | 1:QA:1061:G:C8 | 2.51 | 0.45 |
| 1:QA:56:U:H2' | 1:QA:57:G:H8 | 1.81 | 0.45 |
| 1:QA:59:A:H3' | 1:QA:331:G:H22 | 1.81 | 0.45 |
| 4:QD:98:GLU:HA | 4:QD:103:ASN:HD22 | 1.82 | 0.45 |
| 6:QF:97:PHE:HB2 | 18:QR:32:ARG:HE | 1.81 | 0.45 |
| 53:R8:62:LEU:HA | 53:R8:64:TYR:HD2 | 1.81 | 0.45 |
| 24:RA:1267:U:H2' | 24:RA:1268:A:H8 | 1.81 | 0.45 |
| 24:RA:1302:A:H5' | 24:RA:1608:A:OP2 | 2.16 | 0.45 |
| 24:RA:2021:C:OP1 | 50:R5:12:SER:OG | 2.26 | 0.45 |
| 24:RA:2306:C:H2' | 24:RA:2307:G:N2 | 2.31 | 0.45 |
| 24:RA:784:A:O2' | 24:RA:785:G:H5'' | 2.15 | 0.45 |
| 29:RG:63:ILE:HG13 | 29:RG:64:THR:HG23 | 1.97 | 0.45 |
| 24:RA:2657:A:O2' | 30:RH:160:LYS:NZ | 2.48 | 0.45 |
| 34:RP:115:LEU:HA | 34:RP:134:ALA:HB2 | 1.99 | 0.45 |
| 1:XA:519:C:H2' | 1:XA:520:A:C8 | 2.52 | 0.45 |
| 1:XA:950:U:H2' | 1:XA:951:G:C8 | 2.51 | 0.45 |
| 1:XA:489:C:H5'' | 4:XD:132:ARG:HH22 | 1.81 | 0.45 |
| 4:XD:3:ARG:HD3 | 4:XD:118:ARG:HH21 | 1.80 | 0.45 |
| 48:Y3:40:THR:HG22 | 48:Y3:42:ALA:H | 1.82 | 0.45 |
| 24:YA:1297:C:H2' | 24:YA:1298:C:H6 | 1.81 | 0.45 |
| 24:YA:1336:A:H2' | 24:YA:1337:G:C8 | 2.52 | 0.45 |
| 24:YA:1609:A:N1 | 24:YA:1616:A:C6 | 2.84 | 0.45 |
| 24:YA:231:C:H3' | 24:YA:232:G:C8 | 2.51 | 0.45 |
| 24:YA:2377:A:H2' | 24:YA:2378:A:C8 | 2.51 | 0.45 |
| 24:YA:2546:U:H4' | 24:YA:2566:A:H2 | 1.81 | 0.45 |
| 24:YA:746:A:O2' | 24:YA:2611:U:O2' | 2.25 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:YP:49:ARG:HH11 | 53:Y8:58:ILE:HG22 | 1.80 | 0.45 |
| 1:QA:1443:G:H5' | 1:QA:1446:A:OP2 | 2.17 | 0.45 |
| 1:QA:299:G:H2' | 1:QA:300:A:C8 | 2.52 | 0.45 |
| 12:QL:91:LYS:HA | 12:QL:91:LYS:HD3 | 1.78 | 0.45 |
| 13:QM:39:ILE:HG21 | 13:QM:56:LEU:HD21 | 1.99 | 0.45 |
| 22:QV:24:C:H2' | 22:QV:25:G:C8 | 2.52 | 0.45 |
| 24:RA:1259:G:H2' | 24:RA:1260:G:H8 | 1.81 | 0.45 |
| 24:RA:1292:U:H2' | 24:RA:1293:C:C6 | 2.52 | 0.45 |
| 24:RA:1542:G:H5'' | 24:RA:1543:A:OP2 | 2.17 | 0.45 |
| 24:RA:2537:U:H2' | 24:RA:2538:C:C6 | 2.51 | 0.45 |
| 24:RA:597:U:H2' | 24:RA:598:G:C8 | 2.51 | 0.45 |
| 34:RP:92:GLU:HA | 34:RP:123:LEU:HD11 | 1.98 | 0.45 |
| 1:XA:1469:G:H2' | 1:XA:1470:G:C8 | 2.52 | 0.45 |
| 1:XA:272:C:H2' | 1:XA:273:A:C8 | 2.48 | 0.45 |
| 1:XA:74:C:H2' | 1:XA:75:C:C6 | 2.51 | 0.45 |
| 3:XC:190:ARG:H | 3:XC:195:VAL:HG13 | 1.82 | 0.45 |
| 4:XD:74:GLN:O | 4:XD:78:LEU:HG | 2.16 | 0.45 |
| 11:XK:18:ARG:HG3 | 11:XK:35:PRO:HA | 1.98 | 0.45 |
| 47:Y2:45:SER:OG | 47:Y2:46:GLN:N | 2.49 | 0.45 |
| 24:YA:186:G:H2' | 24:YA:187:G:H8 | 1.81 | 0.45 |
| 24:YA:2591:C:H2' | 24:YA:2592:G:C8 | 2.51 | 0.45 |
| 24:YA:270(U):C:H2' | 24:YA:270(V):G:H8 | 1.82 | 0.45 |
| 24:YA:852:G:H2' | 24:YA:853:G:C8 | 2.52 | 0.45 |
| 1:QA:1066:C:H3' | 1:QA:1067:A:H8 | 1.82 | 0.45 |
| 1:QA:1320:C:O2 | 19:QS:36:ARG:NH2 | 2.50 | 0.45 |
| 1:QA:1469:G:H2' | 1:QA:1470:G:H8 | 1.82 | 0.45 |
| 1:QA:186(F):C:H2' | 1:QA:187:C:O4' | 2.16 | 0.45 |
| 1:QA:7:G:C6 | 1:QA:298:A:C2 | 3.05 | 0.45 |
| 1:QA:924:C:H2' | 1:QA:925:G:C8 | 2.52 | 0.45 |
| 1:QA:976:G:OP2 | 1:QA:1358:U:O2' | 2.34 | 0.45 |
| 2:QB:69:LEU:HD23 | 2:QB:159:PRO:HB3 | 1.98 | 0.45 |
| 4:QD:49:ARG:HD3 | 4:QD:50:ARG:H | 1.81 | 0.45 |
| 9:QI:67:GLY:O | 9:QI:73:GLN:NE2 | 2.50 | 0.45 |
| 49:R4:26:SER:OG | 49:R4:28:LYS:O | 2.34 | 0.45 |
| 24:RA:1065:U:O2 | 24:RA:1074:G:N1 | 2.50 | 0.45 |
| 24:RA:1085:A:O2' | 24:RA:1086:A:OP1 | 2.28 | 0.45 |
| 24:RA:1231:G:H2' | 24:RA:1232:G:H8 | 1.81 | 0.45 |
| 24:RA:2064:C:H2' | 24:RA:2065:C:C6 | 2.51 | 0.45 |
| 24:RA:2183:C:H2' | 24:RA:2184:G:H8 | 1.81 | 0.45 |
| 24:RA:2845:G:H2' | 24:RA:2846:G:H8 | 1.82 | 0.45 |
| 25:RB:28:C:H2' | 25:RB:29:A:C8 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:RB:44:G:H1' | 25:RB:47:C:H42 | 1.81 | 0.45 |
| 32:RN:27:ALA:HA | 32:RN:30:ILE:HD12 | 1.98 | 0.45 |
| 32:RN:6:PRO:HG3 | 32:RN:41:ASP:HB2 | 1.98 | 0.45 |
| 35:RQ:111:GLU:OE1 | 35:RQ:133:ARG:NH2 | 2.50 | 0.45 |
| 1:XA:1256:A:H4' | 1:XA:1258:G:C4 | 2.52 | 0.45 |
| 1:XA:1305:G:O2' | 1:XA:1332:A:N6 | 2.50 | 0.45 |
| 1:XA:1427:U:H2' | 1:XA:1428:A:C8 | 2.52 | 0.45 |
| 1:XA:227:G:H2' | 1:XA:228:A:C8 | 2.51 | 0.45 |
| 1:XA:686:U:H2' | 1:XA:687:A:C8 | 2.52 | 0.45 |
| 1:XA:782:A:H62 | 1:XA:800:G:H21 | 1.65 | 0.45 |
| 9:XI:42:ARG:NH1 | 9:XI:71:SER:OG | 2.49 | 0.45 |
| 53:Y8:62:LEU:HA | 53:Y8:64:TYR:HD1 | 1.81 | 0.45 |
| 24:YA:1063:G:H2' | 24:YA:1064:C:O4' | 2.17 | 0.45 |
| 24:YA:1226:G:OP1 | 40:YV:69:LYS:NZ | 2.45 | 0.45 |
| 24:YA:2059:A:H5' | 24:YA:2060:A:OP2 | 2.17 | 0.45 |
| 24:YA:2215:G:H2' | 24:YA:2216:G:H8 | 1.81 | 0.45 |
| 24:YA:861:A:N3 | 25:YB:79:C:O2' | 2.50 | 0.45 |
| 25:YB:66:A:O2' | 25:YB:67:G:O5' | 2.32 | 0.45 |
| 26:YD:108:PRO:HB3 | 26:YD:143:HIS:CE1 | 2.52 | 0.45 |
| 28:YF:195:ASP:OD1 | 28:YF:195:ASP:N | 2.46 | 0.45 |
| 29:YG:10:LYS:NZ | 29:YG:14:GLU:OE1 | 2.44 | 0.45 |
| 1:QA:113:G:H2' | 1:QA:114:U:C6 | 2.52 | 0.45 |
| 1:QA:1290:G:H4' | 7:QG:37:ASN:HD21 | 1.82 | 0.45 |
| 1:QA:184:G:H2' | 1:QA:185:A:H8 | 1.82 | 0.45 |
| 1:QA:918:A:H2' | 1:QA:919:A:C8 | 2.52 | 0.45 |
| 8:QH:75:ARG:HG2 | 8:QH:75:ARG:H | 1.66 | 0.45 |
| 7:QG:16:LEU:HD21 | 9:QI:45:ALA:N | 2.31 | 0.45 |
| 24:RA:1206:G:H2' | 24:RA:1207:C:C6 | 2.52 | 0.45 |
| 24:RA:1210:A:H4' | 24:RA:1211:U:O5' | 2.16 | 0.45 |
| 24:RA:1592:C:H2' | 24:RA:1593:G:C8 | 2.51 | 0.45 |
| 24:RA:1637:A:H2' | 24:RA:1638:C:C6 | 2.52 | 0.45 |
| 24:RA:1667:G:O2' | 24:RA:1991:U:O4 | 2.34 | 0.45 |
| 24:RA:372:G:O2' | 24:RA:373:U:O5' | 2.32 | 0.45 |
| 25:RB:30:C:O2' | 25:RB:57:A:N1 | 2.50 | 0.45 |
| 27:RE:143:ASN:HB2 | 27:RE:147:PRO:HD2 | 1.99 | 0.45 |
| 36:RR:74:LYS:O | 36:RR:75:LEU:HB3 | 2.16 | 0.45 |
| 44:RZ:13:GLU:HB3 | 44:RZ:18:LEU:HD21 | 1.99 | 0.45 |
| 1:XA:1273:G:H3' | 1:XA:1274:G:C8 | 2.52 | 0.45 |
| 21:XU:10:ARG:HA | 21:XU:13:ILE:HG12 | 1.99 | 0.45 |
| 24:YA:1769:G:H2' | 24:YA:1770:G:H8 | 1.82 | 0.45 |
| 24:YA:2513:G:H2' | 24:YA:2514:U:C6 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1145:C:H4' | 1:QA:1146:A:C8 | 2.52 | 0.45 |
| 1:QA:1349:A:H62 | 1:QA:1373:G:H21 | 1.63 | 0.45 |
| 1:QA:639:G:H2' | 1:QA:640:A:C8 | 2.52 | 0.45 |
| 1:QA:768:A:N3 | 1:QA:1512:U:O2' | 2.50 | 0.45 |
| 3:QC:189:ALA:HB3 | 3:QC:196:LEU:HB2 | 1.99 | 0.45 |
| 13:QM:74:VAL:O | 13:QM:78:ILE:HG12 | 2.16 | 0.45 |
| 24:RA:1152:C:H4' | 39:RU:77:SER:HA | 1.98 | 0.45 |
| 24:RA:1336:A:H2' | 24:RA:1337:G:C8 | 2.52 | 0.45 |
| 24:RA:1569:A:H2' | 24:RA:1570:A:C8 | 2.51 | 0.45 |
| 24:RA:1841:U:H2' | 24:RA:1842:G:H8 | 1.82 | 0.45 |
| 24:RA:2647:U:H2' | 24:RA:2648:C:C6 | 2.52 | 0.45 |
| 24:RA:300:A:P | 43:RY:84:ARG:HH22 | 2.39 | 0.45 |
| 24:RA:2310:A:N6 | 29:RG:79:ASN:OD1 | 2.49 | 0.45 |
| 30:RH:151:ILE:O | 30:RH:153:LYS:N | 2.50 | 0.45 |
| 44:RZ:94:GLU:HG3 | 44:RZ:95:PRO:HD3 | 1.99 | 0.45 |
| 1:XA:1218:C:H2' | 1:XA:1219:U:C6 | 2.52 | 0.45 |
| 1:XA:1315:U:O2' | 1:XA:1360:A:N3 | 2.44 | 0.45 |
| 4:XD:116:GLN:O | 4:XD:120:LEU:HG | 2.17 | 0.45 |
| 5:XE:5:ASP:N | 5:XE:5:ASP:OD1 | 2.50 | 0.45 |
| 7:XG:116:ALA:O | 7:XG:120:ILE:HG12 | 2.16 | 0.45 |
| 18:XR:59:SER:N | 18:XR:62:GLU:OE2 | 2.41 | 0.45 |
| 24:YA:1201:C:H2' | 24:YA:1202:C:H6 | 1.80 | 0.45 |
| 24:YA:2036:C:H2' | 24:YA:2037:G:C8 | 2.51 | 0.45 |
| 24:YA:2466:C:H5'' | 54:Y9:6:SER:HB3 | 1.99 | 0.45 |
| 24:YA:519:U:H2' | 24:YA:520:G:H8 | 1.81 | 0.45 |
| 24:YA:703:U:H3 | 24:YA:728:G:H1 | 1.65 | 0.45 |
| 24:YA:870:A:OP1 | 35:YQ:6:ARG:NH2 | 2.46 | 0.45 |
| 26:YD:17:THR:HB | 26:YD:205:VAL:H | 1.81 | 0.45 |
| 24:YA:2051:A:H4' | 27:YE:141:ILE:HG12 | 1.98 | 0.45 |
| 29:YG:167:GLU:N | 29:YG:167:GLU:OE2 | 2.48 | 0.45 |
| 1:QA:123:C:H2' | 1:QA:124:G:H8 | 1.82 | 0.45 |
| 1:QA:12:U:H4' | 1:QA:526:C:H4' | 1.99 | 0.45 |
| 1:QA:1481:U:H2' | 1:QA:1482:G:C8 | 2.51 | 0.45 |
| 1:QA:281:G:OP2 | 1:QA:281:G:H8 | 2.00 | 0.45 |
| 1:QA:297:G:H4' | 1:QA:557:G:H4' | 1.99 | 0.45 |
| 1:QA:444:C:H2' | 1:QA:445:G:C8 | 2.52 | 0.45 |
| 1:QA:743:U:H2' | 1:QA:744:C:C6 | 2.52 | 0.45 |
| 8:QH:10:LEU:HD21 | 8:QH:85:ARG:HB2 | 1.99 | 0.45 |
| 24:RA:1310:G:OP2 | 52:R7:9:ARG:NE | 2.33 | 0.45 |
| 24:RA:1430:C:H2' | 24:RA:1431:U:C6 | 2.52 | 0.45 |
| 24:RA:212:G:H2' | 24:RA:213:A:C8 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:RA:2867:G:O2' | 24:RA:2868:A:H8 | 2.00 | 0.45 |
| 24:RA:29:U:H2' | 24:RA:30:G:H8 | 1.81 | 0.45 |
| 24:RA:680:G:H2' | 24:RA:681:G:C8 | 2.52 | 0.45 |
| 29:RG:165:THR:HG23 | 29:RG:168:GLU:H | 1.81 | 0.45 |
| 31:RI:14:ASP:C | 31:RI:16:GLY:H | 2.21 | 0.45 |
| 31:RI:58:LEU:HA | 31:RI:61:ARG:HE | 1.80 | 0.45 |
| 32:RN:34:LEU:O | 32:RN:49:GLY:HA3 | 2.17 | 0.45 |
| 36:RR:45:ARG:HH21 | 36:RR:97:VAL:HG21 | 1.81 | 0.45 |
| 40:RV:43:GLU:HG3 | 40:RV:44:LYS:H | 1.82 | 0.45 |
| 44:RZ:163:LEU:HD22 | 44:RZ:167:PRO:HG3 | 1.98 | 0.45 |
| 1:XA:1510:U:H2' | 1:XA:1511:G:H8 | 1.82 | 0.45 |
| 10:XJ:69:ASN:O | 10:XJ:70:ARG:NE | 2.49 | 0.45 |
| 45:Y0:10:THR:HG22 | 45:Y0:12:ASN:H | 1.82 | 0.45 |
| 24:YA:1359:A:N6 | 24:YA:1372:U:C2 | 2.85 | 0.45 |
| 24:YA:48:G:N2 | 24:YA:177:G:OP2 | 2.50 | 0.45 |
| 24:YA:2629:A:O2' | 24:YA:2630:G:H5'' | 2.17 | 0.45 |
| 24:YA:262:A:N3 | 24:YA:430:G:O2' | 2.34 | 0.45 |
| 24:YA:270(U):C:H2' | 24:YA:270(V):G:C8 | 2.52 | 0.45 |
| 24:YA:436:C:H2' | 24:YA:438:G:C8 | 2.51 | 0.45 |
| 24:YA:729:G:C5 | 26:YD:208:LYS:HB2 | 2.52 | 0.45 |
| 27:YE:92:THR:OG1 | 27:YE:93:VAL:N | 2.49 | 0.45 |
| 29:YG:118:ARG:HG3 | 29:YG:181:ARG:HD3 | 1.98 | 0.45 |
| 29:YG:3:LEU:HA | 29:YG:3:LEU:HD12 | 1.83 | 0.45 |
| 30:YH:88:LEU:HA | 30:YH:130:ARG:HA | 1.99 | 0.45 |
| 1:QA:434:U:H2' | 1:QA:435:C:C6 | 2.52 | 0.44 |
| 4:QD:9:CYS:SG | 4:QD:25:ARG:NH1 | 2.83 | 0.44 |
| 9:QI:64:THR:OG1 | 9:QI:64:THR:O | 2.34 | 0.44 |
| 1:QA:1227:A:H5'' | 13:QM:111:LYS:NZ | 2.32 | 0.44 |
| 13:QM:47:ASP:N | 13:QM:47:ASP:OD1 | 2.47 | 0.44 |
| 24:RA:1107:G:H2' | 24:RA:1108:U:H6 | 1.82 | 0.44 |
| 24:RA:1927:A:H2' | 24:RA:1928:A:C8 | 2.52 | 0.44 |
| 24:RA:2647:U:H2' | 24:RA:2648:C:H6 | 1.82 | 0.44 |
| 24:RA:872:A:H2' | 24:RA:873:G:C8 | 2.52 | 0.44 |
| 29:RG:125:PHE:HD2 | 29:RG:166:ASP:HB2 | 1.81 | 0.44 |
| 30:RH:85:LYS:HB3 | 30:RH:133:VAL:HB | 1.98 | 0.44 |
| 24:RA:660:G:H21 | 34:RP:12:ALA:HA | 1.81 | 0.44 |
| 34:RP:37:GLY:N | 34:RP:40:SER:OG | 2.50 | 0.44 |
| 37:RS:42:ASP:O | 37:RS:43:GLU:HG2 | 2.17 | 0.44 |
| 44:RZ:4:ARG:HA | 44:RZ:59:LEU:H | 1.83 | 0.44 |
| 1:XA:1268:A:H2' | 1:XA:1269:A:C8 | 2.52 | 0.44 |
| 1:XA:1277:C:O2' | 1:XA:1279:A:H1' | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:704:A:H8 | 1:XA:704:A:OP2 | 2.00 | 0.44 |
| 1:XA:97:U:H2' | 1:XA:99:C:C6 | 2.52 | 0.44 |
| 4:XD:122:ARG:HD3 | 4:XD:136:PRO:HD3 | 2.00 | 0.44 |
| 13:XM:3:ARG:O | 13:XM:57:ARG:NH1 | 2.50 | 0.44 |
| 24:YA:1113:U:H2' | 24:YA:1114:G:H8 | 1.82 | 0.44 |
| 24:YA:1292:U:H2' | 24:YA:1293:C:H6 | 1.82 | 0.44 |
| 24:YA:1923:U:H2' | 24:YA:1924:C:C6 | 2.52 | 0.44 |
| 24:YA:198:C:O2' | 24:YA:199:A:H5' | 2.17 | 0.44 |
| 25:YB:3:C:H2' | 25:YB:4:C:C6 | 2.52 | 0.44 |
| 25:YB:87:G:H22 | 25:YB:89:G:H3' | 1.81 | 0.44 |
| 25:YB:9:G:OP1 | 37:YS:15:ARG:NH1 | 2.36 | 0.44 |
| 26:YD:254:THR:O | 26:YD:254:THR:OG1 | 2.35 | 0.44 |
| 27:YE:69:LYS:HA | 27:YE:69:LYS:HD3 | 1.76 | 0.44 |
| 38:YT:30:VAL:HG23 | 38:YT:86:ILE:HB | 1.98 | 0.44 |
| 41:YW:35:ILE:O | 41:YW:39:THR:OG1 | 2.33 | 0.44 |
| 43:YY:14:LEU:HB2 | 43:YY:75:ILE:HD11 | 1.98 | 0.44 |
| 1:QA:1376:U:H2' | 1:QA:1377:A:C8 | 2.52 | 0.44 |
| 1:QA:1419:G:H1 | 1:QA:1481:U:H3 | 1.63 | 0.44 |
| 1:QA:555:C:H2' | 1:QA:556:C:C6 | 2.52 | 0.44 |
| 1:QA:851:G:H2' | 1:QA:852:G:H8 | 1.80 | 0.44 |
| 3:QC:95:THR:HG22 | 3:QC:97:LYS:H | 1.82 | 0.44 |
| 4:QD:131:ARG:NH1 | 4:QD:132:ARG:O | 2.50 | 0.44 |
| 9:QI:17:VAL:HG22 | 9:QI:63:ILE:HD12 | 1.99 | 0.44 |
| 24:RA:1408:C:H2' | 24:RA:1409:C:C6 | 2.52 | 0.44 |
| 24:RA:1899:G:O2' | 24:RA:1900:A:H5'' | 2.17 | 0.44 |
| 24:RA:2121:G:H2' | 24:RA:2122:U:C6 | 2.53 | 0.44 |
| 24:RA:2674:G:H2' | 24:RA:2675:A:C8 | 2.53 | 0.44 |
| 24:RA:2857:G:N2 | 24:RA:2859:G:H3' | 2.32 | 0.44 |
| 24:RA:39:C:H2' | 24:RA:40:C:C6 | 2.52 | 0.44 |
| 24:RA:574:C:O2 | 27:RE:145:LYS:NZ | 2.50 | 0.44 |
| 24:RA:724:U:H2' | 24:RA:725:G:O4' | 2.17 | 0.44 |
| 24:RA:872:A:H2' | 24:RA:873:G:H8 | 1.82 | 0.44 |
| 24:RA:900:A:H3' | 24:RA:901:A:H8 | 1.82 | 0.44 |
| 28:RF:11:VAL:HG21 | 28:RF:20:LEU:HD23 | 1.99 | 0.44 |
| 35:RQ:60:ARG:HH22 | 44:RZ:113:ALA:HB3 | 1.81 | 0.44 |
| 37:RS:16:ASN:OD1 | 37:RS:19:LYS:NZ | 2.50 | 0.44 |
| 24:YA:1341:U:OP1 | 24:YA:1397:U:N3 | 2.35 | 0.44 |
| 24:YA:2246:G:H2' | 24:YA:2247:A:C8 | 2.52 | 0.44 |
| 24:YA:2577:A:O4' | 50:Y5:3:LYS:HB2 | 2.17 | 0.44 |
| 24:YA:2836:U:H2' | 24:YA:2837:G:H8 | 1.82 | 0.44 |
| 24:YA:841:A:H2' | 24:YA:842:G:H8 | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:YA:923:C:H2' | 24:YA:924:C:C6 | 2.53 | 0.44 |
| 34:YP:84:ASN:HA | 34:YP:115:LEU:O | 2.18 | 0.44 |
| 1:QA:1004:A:P | 1:QA:1025:U:H3 | 2.40 | 0.44 |
| 1:QA:328:C:H1' | 1:QA:329:A:OP2 | 2.17 | 0.44 |
| 4:QD:68:TYR:CD2 | 4:QD:97:LEU:HD12 | 2.53 | 0.44 |
| 11:QK:96:ARG:HA | 11:QK:99:GLN:HE21 | 1.82 | 0.44 |
| 54:R9:27:CYS:SG | 54:R9:28:GLU:N | 2.91 | 0.44 |
| 24:RA:1389:G:H2' | 24:RA:1390:U:C6 | 2.52 | 0.44 |
| 24:RA:2487:G:H2' | 24:RA:2488:A:C8 | 2.52 | 0.44 |
| 24:RA:635:C:H2' | 24:RA:636:G:O4' | 2.17 | 0.44 |
| 24:RA:678:C:H2' | 24:RA:679:C:H6 | 1.81 | 0.44 |
| 24:RA:923:C:H2' | 24:RA:924:C:H6 | 1.82 | 0.44 |
| 24:RA:948:G:H2' | 24:RA:949:C:H6 | 1.82 | 0.44 |
| 24:RA:661:C:H5'' | 34:RP:15:ARG:NH2 | 2.31 | 0.44 |
| 1:XA:1314:C:H2' | 1:XA:1315:U:C6 | 2.52 | 0.44 |
| 1:XA:1404:C:H2' | 1:XA:1405:G:C8 | 2.53 | 0.44 |
| 1:XA:312:C:H2' | 1:XA:313:A:H8 | 1.82 | 0.44 |
| 1:XA:109:A:C6 | 1:XA:326:G:C6 | 3.05 | 0.44 |
| 1:XA:505:G:H2' | 1:XA:506:G:C8 | 2.52 | 0.44 |
| 1:XA:985:C:H2' | 1:XA:986:A:H8 | 1.82 | 0.44 |
| 2:XB:43:ASP:O | 2:XB:47:THR:OG1 | 2.33 | 0.44 |
| 22:XV:1:C:H2' | 22:XV:2:G:H8 | 1.81 | 0.44 |
| 45:Y0:38:VAL:HG21 | 45:Y0:45:PHE:HD2 | 1.83 | 0.44 |
| 24:YA:1625:C:H2' | 24:YA:1626:G:O4' | 2.18 | 0.44 |
| 24:YA:1657:C:H2' | 24:YA:1658:C:H6 | 1.82 | 0.44 |
| 24:YA:1657:C:H2' | 24:YA:1658:C:C6 | 2.52 | 0.44 |
| 24:YA:1889:A:H2' | 24:YA:1890:A:C8 | 2.51 | 0.44 |
| 24:YA:2364:C:H2' | 24:YA:2365:G:O4' | 2.17 | 0.44 |
| 24:YA:970:C:H2' | 24:YA:971:C:C6 | 2.53 | 0.44 |
| 1:QA:1175:G:H2' | 1:QA:1176:A:C8 | 2.53 | 0.44 |
| 1:QA:1400:C:C4' | 23:QX:21:G:C6 | 3.00 | 0.44 |
| 1:QA:1516:G:H2' | 1:QA:1518:A:OP2 | 2.17 | 0.44 |
| 13:QM:18:ALA:HA | 13:QM:21:TYR:HD2 | 1.83 | 0.44 |
| 10:QJ:51:ARG:O | 14:QN:45:ARG:NH1 | 2.50 | 0.44 |
| 15:QO:67:LEU:HD12 | 15:QO:78:TYR:CE1 | 2.53 | 0.44 |
| 24:RA:1140:C:OP1 | 32:RN:23:LEU:HB3 | 2.17 | 0.44 |
| 24:RA:1181:C:H2' | 24:RA:1182:A:C8 | 2.52 | 0.44 |
| 24:RA:1205:U:C4 | 28:RF:171:PRO:HA | 2.53 | 0.44 |
| 24:RA:1812:A:H2' | 24:RA:1813:G:H8 | 1.82 | 0.44 |
| 24:RA:20:C:H2' | 24:RA:21:A:H8 | 1.82 | 0.44 |
| 24:RA:2564:A:H2' | 24:RA:2565:A:C8 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:RA:956:G:H2' | 24:RA:957:A:H2' | 1.99 | 0.44 |
| 30:RH:67:LEU:O | 30:RH:71:LEU:HG | 2.18 | 0.44 |
| 36:RR:38:VAL:HG22 | 36:RR:112:ALA:HB2 | 1.98 | 0.44 |
| 40:RV:44:LYS:HB3 | 40:RV:45:THR:H | 1.52 | 0.44 |
| 42:RX:21:PHE:HA | 42:RX:26:TYR:HE1 | 1.80 | 0.44 |
| 1:XA:107:G:H3' | 1:XA:108:G:H21 | 1.82 | 0.44 |
| 1:XA:1238:A:H62 | 1:XA:1301:U:H3 | 1.65 | 0.44 |
| 1:XA:161:A:H2' | 1:XA:162:A:C8 | 2.53 | 0.44 |
| 1:XA:812:C:H1' | 1:XA:813:U:OP2 | 2.18 | 0.44 |
| 5:XE:103:GLY:C | 5:XE:106:PRO:HD2 | 2.38 | 0.44 |
| 5:XE:89:ILE:HD12 | 5:XE:121:LYS:O | 2.18 | 0.44 |
| 24:YA:1332:G:H8 | 24:YA:1332:G:H2' | 1.59 | 0.44 |
| 24:YA:177:G:H3' | 24:YA:178:G:H8 | 1.81 | 0.44 |
| 24:YA:2025:C:H2' | 24:YA:2026:C:C6 | 2.52 | 0.44 |
| 24:YA:247:G:H4' | 24:YA:386:G:C5 | 2.52 | 0.44 |
| 24:YA:659:C:H2' | 24:YA:660:G:C8 | 2.53 | 0.44 |
| 24:YA:956:G:OP2 | 35:YQ:85:LYS:NZ | 2.50 | 0.44 |
| 31:YI:30:LEU:HB3 | 31:YI:36:ALA:HB3 | 1.98 | 0.44 |
| 32:YN:34:LEU:HA | 32:YN:34:LEU:HD13 | 1.77 | 0.44 |
| 38:YT:16:ARG:HH21 | 38:YT:19:LEU:HD21 | 1.83 | 0.44 |
| 39:YU:50:ARG:O | 39:YU:54:LYS:NZ | 2.51 | 0.44 |
| 1:QA:1032(A):G:H2' | 1:QA:1032(B):G:C8 | 2.51 | 0.44 |
| 1:QA:243:A:H4' | 1:QA:244:U:H3' | 2.00 | 0.44 |
| 1:QA:626:U:P | 16:QP:18:ARG:HH21 | 2.40 | 0.44 |
| 1:QA:707:C:H4' | 11:QK:20:TYR:HD2 | 1.82 | 0.44 |
| 14:QN:39:LEU:HD23 | 14:QN:39:LEU:HA | 1.89 | 0.44 |
| 18:QR:32:ARG:HA | 18:QR:69:THR:HG21 | 1.99 | 0.44 |
| 1:QA:719:C:H1' | 18:QR:49:LYS:HG2 | 1.99 | 0.44 |
| 24:RA:2020:A:N7 | 50:R5:9:LYS:NZ | 2.66 | 0.44 |
| 24:RA:16:G:H2' | 24:RA:17:G:H8 | 1.82 | 0.44 |
| 24:RA:2292:C:H2' | 24:RA:2293:C:C6 | 2.52 | 0.44 |
| 24:RA:2306:C:OP2 | 24:RA:2307:G:H2' | 2.18 | 0.44 |
| 24:RA:2546:U:H5'' | 24:RA:2547:U:H5' | 1.99 | 0.44 |
| 24:RA:2554:U:H2' | 24:RA:2555:U:C6 | 2.53 | 0.44 |
| 24:RA:2791:C:H4' | 24:RA:2792:G:H5' | 2.00 | 0.44 |
| 24:RA:832:G:H2' | 24:RA:833:U:C6 | 2.53 | 0.44 |
| 26:RD:108:PRO:HB3 | 26:RD:143:HIS:CE1 | 2.53 | 0.44 |
| 33:RO:24:VAL:HG12 | 33:RO:33:ALA:HB2 | 1.99 | 0.44 |
| 36:RR:74:LYS:HD2 | 36:RR:74:LYS:HA | 1.77 | 0.44 |
| 1:XA:116:A:C8 | 1:XA:116:A:OP2 | 2.70 | 0.44 |
| 1:XA:768:A:H4' | 1:XA:1523:G:N2 | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:288:A:H2' | 1:XA:289:G:H4' | 1.98 | 0.44 |
| 1:XA:381:C:H2' | 1:XA:382:A:O4' | 2.17 | 0.44 |
| 1:XA:390:C:H2' | 1:XA:391:G:C8 | 2.53 | 0.44 |
| 1:XA:966:G:C2 | 22:XV:35:C:H5' | 2.52 | 0.44 |
| 34:YP:62:LEU:HD12 | 53:Y8:30:ARG:HE | 1.82 | 0.44 |
| 53:Y8:7:HIS:HB3 | 53:Y8:59:LYS:HG2 | 1.98 | 0.44 |
| 24:YA:330:A:H2 | 24:YA:1210:A:O2' | 2.01 | 0.44 |
| 24:YA:1394:U:O2 | 42:YX:16:LYS:NZ | 2.50 | 0.44 |
| 24:YA:507:A:H5'' | 24:YA:508:G:H5' | 2.00 | 0.44 |
| 24:YA:608:A:H2' | 24:YA:609:A:C8 | 2.52 | 0.44 |
| 1:QA:1002:G:H2' | 1:QA:1003:G:C8 | 2.53 | 0.44 |
| 1:QA:1304:G:N2 | 1:QA:1334:G:O6 | 2.50 | 0.44 |
| 1:QA:1512:U:H2' | 1:QA:1513:A:H8 | 1.83 | 0.44 |
| 1:QA:34:C:H2' | 1:QA:35:G:C8 | 2.51 | 0.44 |
| 1:QA:422:C:H4' | 1:QA:423:G:C4 | 2.52 | 0.44 |
| 1:QA:690:G:H22 | 11:QK:55:LYS:HZ1 | 1.66 | 0.44 |
| 3:QC:174:PRO:O | 3:QC:177:THR:OG1 | 2.35 | 0.44 |
| 6:QF:35:ALA:HB1 | 6:QF:65:VAL:HG21 | 2.00 | 0.44 |
| 9:QI:2:GLU:HG2 | 9:QI:20:ARG:CZ | 2.47 | 0.44 |
| 20:QT:48:LYS:HD2 | 20:QT:51:GLU:HB2 | 2.00 | 0.44 |
| 23:QX:8:A:H2' | 23:QX:9:G:H8 | 1.80 | 0.44 |
| 24:RA:1000:A:H2' | 24:RA:1001:A:C8 | 2.52 | 0.44 |
| 24:RA:1149:G:H2' | 24:RA:1150:C:C6 | 2.53 | 0.44 |
| 24:RA:144:C:H2' | 24:RA:145:G:C8 | 2.52 | 0.44 |
| 24:RA:1478:G:H1' | 24:RA:1557:C:O2' | 2.18 | 0.44 |
| 24:RA:1496:A:H8 | 24:RA:1577:C:HO2' | 1.66 | 0.44 |
| 24:RA:1657:C:O2' | 27:RE:133:LYS:CD | 2.59 | 0.44 |
| 24:RA:1794:U:H2' | 24:RA:1795:C:C6 | 2.53 | 0.44 |
| 24:RA:1796:U:H2' | 24:RA:1797:C:C6 | 2.52 | 0.44 |
| 24:RA:1800:C:C2 | 24:RA:1802:A:C8 | 3.05 | 0.44 |
| 24:RA:270(U):C:H2' | 24:RA:270(V):G:H8 | 1.82 | 0.44 |
| 24:RA:806:C:O2 | 24:RA:2444:G:O2' | 2.33 | 0.44 |
| 26:RD:79:VAL:HG21 | 26:RD:111:LEU:HD21 | 2.00 | 0.44 |
| 31:RI:79:ILE:HB | 31:RI:142:VAL:HA | 1.98 | 0.44 |
| 32:RN:30:ILE:O | 32:RN:34:LEU:HG | 2.18 | 0.44 |
| 36:RR:74:LYS:C | 36:RR:76:VAL:H | 2.21 | 0.44 |
| 1:XA:1285:A:H1' | 1:XA:1286:A:OP2 | 2.17 | 0.44 |
| 1:XA:944:G:N1 | 1:XA:1338:G:OP2 | 2.33 | 0.44 |
| 8:XH:79:VAL:HG13 | 8:XH:80:ILE:HD12 | 1.99 | 0.44 |
| 51:Y6:23:THR:OG1 | 51:Y6:24:GLU:N | 2.50 | 0.44 |
| 24:YA:1259:G:H2' | 24:YA:1260:G:C8 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 24:YA:144:C:H2' | 24:YA:145:G:C8 | 2.52 | 0.44 |
| 24:YA:2804:C:H2' | 24:YA:2805:G:H8 | 1.82 | 0.44 |
| 24:YA:300:A:OP2 | 43:YY:84:ARG:NH2 | 2.41 | 0.44 |
| 24:YA:816:C:O2' | 24:YA:932:G:O6 | 2.36 | 0.44 |
| 27:YE:31:CYS:HB3 | 27:YE:49:LEU:HG | 1.99 | 0.44 |
| 29:YG:86:MET:HB3 | 29:YG:86:MET:HE2 | 1.75 | 0.44 |
| 1:QA:1010:G:H2' | 1:QA:1011:G:C8 | 2.51 | 0.44 |
| 1:QA:1120:G:H2' | 1:QA:1121:U:C6 | 2.52 | 0.44 |
| 1:QA:997:U:H2' | 1:QA:998:G:C8 | 2.53 | 0.44 |
| 2:QB:75:LYS:HB3 | 2:QB:75:LYS:HE3 | 1.84 | 0.44 |
| 4:QD:208:SER:O | 4:QD:208:SER:OG | 2.35 | 0.44 |
| 4:QD:85:LYS:HD3 | 4:QD:86:LYS:H | 1.83 | 0.44 |
| 5:QE:140:ARG:NH1 | 8:QH:77:GLU:OE1 | 2.51 | 0.44 |
| 6:QF:18:GLN:HA | 6:QF:21:LEU:HB2 | 1.98 | 0.44 |
| 12:QL:84:LEU:O | 12:QL:100:ILE:HD12 | 2.18 | 0.44 |
| 24:RA:1259:G:H2' | 24:RA:1260:G:C8 | 2.52 | 0.44 |
| 24:RA:1571:A:H2' | 24:RA:1572:A:C8 | 2.53 | 0.44 |
| 24:RA:1639:U:C2' | 24:RA:1640:C:H5'' | 2.48 | 0.44 |
| 24:RA:172:C:H2' | 24:RA:173:G:C8 | 2.53 | 0.44 |
| 24:RA:193:U:N3 | 24:RA:203:C:O2 | 2.51 | 0.44 |
| 24:RA:2187:G:H2' | 24:RA:2188:C:C6 | 2.52 | 0.44 |
| 24:RA:250:G:OP2 | 34:RP:59:LEU:HD11 | 2.17 | 0.44 |
| 24:RA:2756:U:OP2 | 54:R9:19:ARG:NE | 2.50 | 0.44 |
| 24:RA:49:A:H61 | 24:RA:177:G:H2' | 1.83 | 0.44 |
| 26:RD:25:THR:O | 26:RD:27:THR:N | 2.50 | 0.44 |
| 1:XA:1241:G:H2' | 1:XA:1242:C:C6 | 2.52 | 0.44 |
| 1:XA:1422:G:H2' | 1:XA:1423:G:H8 | 1.82 | 0.44 |
| 1:XA:464:G:N1 | 1:XA:467:G:OP2 | 2.40 | 0.44 |
| 4:XD:154:ASN:OD1 | 4:XD:154:ASN:N | 2.44 | 0.44 |
| 5:XE:84:PHE:O | 5:XE:87:SER:OG | 2.35 | 0.44 |
| 23:XX:16:C:C5 | 23:XX:16:C:OP2 | 2.70 | 0.44 |
| 23:XX:16:C:C6 | 23:XX:16:C:O5' | 2.70 | 0.44 |
| 24:YA:1012:U:OP1 | 39:YU:75:ASN:ND2 | 2.42 | 0.44 |
| 24:YA:1375:C:H2' | 24:YA:1376:C:H6 | 1.83 | 0.44 |
| 24:YA:1754:C:P | 38:YT:96:ARG:HH12 | 2.41 | 0.44 |
| 24:YA:2151:G:H2' | 24:YA:2152:G:C8 | 2.50 | 0.44 |
| 24:YA:2335:A:O2' | 24:YA:2336:A:H2' | 2.18 | 0.44 |
| 24:YA:2712:U:OP1 | 24:YA:2714:G:H4' | 2.18 | 0.44 |
| 24:YA:433:C:H2' | 24:YA:434:U:C6 | 2.52 | 0.44 |
| 24:YA:639:U:H2' | 24:YA:640:C:H6 | 1.82 | 0.44 |
| 24:YA:829:A:N7 | 24:YA:2247:A:O2' | 2.46 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:YI:123:LEU:HD23 | 31:YI:142:VAL:HG13 | 2.00 | 0.44 |
| 35:YQ:12:GLN:HB2 | 35:YQ:73:PRO:HD2 | 2.00 | 0.44 |
| 1:QA:1054:C:O2 | 1:QA:1196:U:N3 | 2.51 | 0.44 |
| 1:QA:1198:G:H2' | 1:QA:1199:U:C6 | 2.53 | 0.44 |
| 1:QA:277:C:OP2 | 17:QQ:41:LYS:NZ | 2.51 | 0.44 |
| 1:QA:406:G:H2' | 1:QA:407:G:H8 | 1.83 | 0.44 |
| 1:QA:436:C:H2' | 1:QA:437:U:C6 | 2.53 | 0.44 |
| 1:QA:738:C:H2' | 1:QA:739:C:C6 | 2.53 | 0.44 |
| 1:QA:864:A:H2' | 1:QA:865:A:C8 | 2.53 | 0.44 |
| 7:QG:50:ILE:HG21 | 7:QG:61:VAL:HG11 | 2.00 | 0.44 |
| 14:QN:24:CYS:HB3 | 14:QN:27:CYS:SG | 2.56 | 0.44 |
| 51:R6:11:LEU:HB2 | 51:R6:21:TYR:HB2 | 2.00 | 0.44 |
| 24:RA:1821:A:H2' | 24:RA:1822:G:H8 | 1.83 | 0.44 |
| 24:RA:2773:C:H2' | 24:RA:2774:C:H6 | 1.83 | 0.44 |
| 24:RA:831:G:O2' | 34:RP:38:GLN:OE1 | 2.35 | 0.44 |
| 35:RQ:45:GLN:NE2 | 35:RQ:91:GLU:O | 2.51 | 0.44 |
| 37:RS:83:LYS:HD3 | 37:RS:84:GLN:HG3 | 1.99 | 0.44 |
| 41:RW:88:ARG:NH1 | 41:RW:94:ASP:OD1 | 2.50 | 0.44 |
| 1:XA:401:C:H2' | 1:XA:402:G:C8 | 2.53 | 0.44 |
| 1:XA:822:C:H2' | 1:XA:823:G:H8 | 1.83 | 0.44 |
| 7:XG:72:ARG:O | 7:XG:91:VAL:HG22 | 2.17 | 0.44 |
| 1:XA:265:G:H4' | 17:XQ:66:SER:HA | 2.00 | 0.44 |
| 45:Y0:32:ARG:N | 45:Y0:35:ASN:OD1 | 2.49 | 0.44 |
| 24:YA:1542:G:H5'' | 24:YA:1543:A:OP2 | 2.18 | 0.44 |
| 24:YA:1636:C:H2' | 24:YA:1637:A:H8 | 1.82 | 0.44 |
| 24:YA:1694:C:H1' | 24:YA:1695:G:OP2 | 2.18 | 0.44 |
| 24:YA:2692:C:H2' | 24:YA:2693:A:C8 | 2.52 | 0.44 |
| 24:YA:428:A:H3' | 24:YA:429:A:C8 | 2.53 | 0.44 |
| 24:YA:639:U:H2' | 24:YA:640:C:C6 | 2.52 | 0.44 |
| 24:YA:742:G:H2' | 24:YA:743:G:H8 | 1.83 | 0.44 |
| 24:YA:1568:G:H5'' | 26:YD:61:LEU:HD23 | 2.00 | 0.44 |
| 27:YE:24:THR:OG1 | 27:YE:186:GLY:HA2 | 2.18 | 0.44 |
| 29:YG:24:GLY:O | 29:YG:26:GLN:NE2 | 2.50 | 0.44 |
| 32:YN:30:ILE:HG23 | 32:YN:52:VAL:HG11 | 2.00 | 0.44 |
| 33:YO:23:ARG:NH2 | 33:YO:28:SER:O | 2.50 | 0.44 |
| 43:YY:33:LYS:HG3 | 43:YY:34:LYS:HD2 | 1.99 | 0.44 |
| 1:QA:337:C:H2' | 1:QA:338:A:C8 | 2.53 | 0.44 |
| 1:QA:360:A:H2' | 1:QA:361:G:C8 | 2.52 | 0.44 |
| 3:QC:189:ALA:O | 3:QC:190:ARG:HD3 | 2.18 | 0.44 |
| 5:QE:121:LYS:HZ3 | 5:QE:122:GLU:H | 1.65 | 0.44 |
| 5:QE:78:HIS:HB3 | 8:QH:107:LEU:HD12 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:QG:94:ARG:NH1 | 7:QG:98:SER:OG | 2.51 | 0.44 |
| 10:QJ:39:PRO:HA | 10:QJ:70:ARG:HD3 | 2.00 | 0.44 |
| 14:QN:27:CYS:SG | 14:QN:28:GLY:N | 2.91 | 0.44 |
| 24:RA:1431:U:H2' | 24:RA:1432:C:C6 | 2.53 | 0.44 |
| 24:RA:1467:C:H5 | 24:RA:1546:C:H2' | 1.82 | 0.44 |
| 24:RA:2236:C:H2' | 24:RA:2237:G:O4' | 2.18 | 0.44 |
| 24:RA:2646:C:OP2 | 24:RA:2732:G:O2' | 2.28 | 0.44 |
| 24:RA:307:G:C8 | 24:RA:307:G:C3' | 3.00 | 0.44 |
| 24:RA:778:G:H5' | 26:RD:48:ARG:HE | 1.83 | 0.44 |
| 24:RA:864:G:H2' | 24:RA:865:C:C6 | 2.53 | 0.44 |
| 26:RD:85:ASP:OD2 | 26:RD:88:ARG:NH1 | 2.41 | 0.44 |
| 24:RA:631:A:H5' | 34:RP:65:ARG:HD3 | 2.00 | 0.44 |
| 24:RA:906:G:O2' | 35:RQ:67:ARG:NH2 | 2.51 | 0.44 |
| 35:RQ:68:ILE:HD13 | 35:RQ:103:MET:HG2 | 2.00 | 0.44 |
| 40:RV:40:LEU:HD11 | 40:RV:47:VAL:HG12 | 1.99 | 0.44 |
| 1:XA:1502:A:H2' | 1:XA:1504:G:N7 | 2.33 | 0.44 |
| 1:XA:191(D):U:H2' | 1:XA:191(E):G:C8 | 2.52 | 0.44 |
| 1:XA:299:G:H2' | 1:XA:300:A:C8 | 2.53 | 0.44 |
| 1:XA:825:G:H2' | 1:XA:826:C:C6 | 2.53 | 0.44 |
| 1:XA:952:U:H2' | 1:XA:953:G:C8 | 2.53 | 0.44 |
| 4:XD:13:ARG:HB2 | 4:XD:40:PRO:HD3 | 2.00 | 0.44 |
| 14:XN:46:GLU:HG3 | 14:XN:47:LEU:HD22 | 1.99 | 0.44 |
| 50:Y5:36:CYS:CB | 50:Y5:49:CYS:HB3 | 2.48 | 0.44 |
| 24:YA:2549:G:H2' | 24:YA:2550:G:H8 | 1.83 | 0.44 |
| 24:YA:71:A:N3 | 24:YA:73:A:N6 | 2.66 | 0.44 |
| 24:YA:922:U:H2' | 24:YA:923:C:H6 | 1.83 | 0.44 |
| 28:YF:125:LEU:HA | 28:YF:194:MET:O | 2.17 | 0.44 |
| 31:YI:14:ASP:O | 31:YI:16:GLY:N | 2.43 | 0.44 |
| 35:YQ:111:GLU:OE1 | 35:YQ:133:ARG:NH2 | 2.51 | 0.44 |
| 43:YY:37:VAL:HG11 | 43:YY:72:VAL:HG11 | 2.00 | 0.44 |
| 1:QA:106:C:H2' | 1:QA:107:G:C8 | 2.53 | 0.43 |
| 1:QA:1124:G:H3' | 1:QA:1145:C:N4 | 2.33 | 0.43 |
| 1:QA:1320:C:H2' | 1:QA:1321:C:C6 | 2.53 | 0.43 |
| 1:QA:1329:A:H5'' | 13:QM:26:GLY:H | 1.83 | 0.43 |
| 1:QA:1342:C:H1' | 9:QI:124:GLN:HE22 | 1.83 | 0.43 |
| 1:QA:1466:C:H2' | 1:QA:1467:G:O4' | 2.18 | 0.43 |
| 1:QA:1510:U:H3 | 1:QA:1525:G:H1 | 1.65 | 0.43 |
| 1:QA:1516:G:N1 | 1:QA:1519:A:OP2 | 2.51 | 0.43 |
| 1:QA:484:G:H4' | 1:QA:485:G:O5' | 2.17 | 0.43 |
| 1:QA:575:G:O2' | 1:QA:821:G:H5' | 2.18 | 0.43 |
| 1:QA:1249:C:O2' | 9:QI:68:GLY:O | 2.29 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:QK:121:PRO:O | 11:QK:126:ARG:NH1 | 2.42 | 0.43 |
| 13:QM:22:ILE:CD1 | 13:QM:22:ILE:N | 2.79 | 0.43 |
| 15:QO:33:THR:HG21 | 15:QO:85:LEU:HD12 | 1.99 | 0.43 |
| 24:RA:1009:A:OP2 | 24:RA:1010:A:OP2 | 2.36 | 0.43 |
| 24:RA:1458:C:H4' | 24:RA:1459:G:O4' | 2.18 | 0.43 |
| 24:RA:1521:G:H5'' | 24:RA:1521:G:C8 | 2.49 | 0.43 |
| 24:RA:2676:C:H2' | 24:RA:2677:G:H8 | 1.83 | 0.43 |
| 24:RA:2740:A:H2' | 24:RA:2741:A:C8 | 2.52 | 0.43 |
| 24:RA:823:G:H2' | 24:RA:824:A:C8 | 2.53 | 0.43 |
| 1:XA:952:U:H2' | 1:XA:953:G:H8 | 1.83 | 0.43 |
| 3:XC:58:GLU:HB2 | 3:XC:65:ALA:HB3 | 1.99 | 0.43 |
| 5:XE:12:LEU:HB3 | 5:XE:31:LEU:HB3 | 1.98 | 0.43 |
| 13:XM:105:THR:OG1 | 13:XM:106:ASN:N | 2.42 | 0.43 |
| 14:YN:27:CYS:SG | 14:YN:28:GLY:N | 2.91 | 0.43 |
| 17:XQ:21:VAL:HG11 | 17:XQ:59:ILE:HG21 | 1.99 | 0.43 |
| 17:XQ:81:ARG:HD3 | 17:XQ:81:ARG:HA | 1.72 | 0.43 |
| 18:XR:53:ARG:HA | 18:XR:56:THR:HG22 | 2.00 | 0.43 |
| 19:XS:81:ARG:HA | 19:XS:81:ARG:HD2 | 1.75 | 0.43 |
| 24:YA:1265:A:H8 | 24:YA:1265:A:OP1 | 2.01 | 0.43 |
| 24:YA:1267:U:H2' | 24:YA:1268:A:H8 | 1.83 | 0.43 |
| 24:YA:2630:G:H2' | 24:YA:2631:G:H8 | 1.82 | 0.43 |
| 24:YA:303:U:H2' | 24:YA:304:G:C8 | 2.53 | 0.43 |
| 24:YA:52:A:OP2 | 24:YA:117:G:N1 | 2.49 | 0.43 |
| 25:YB:60:C:H2' | 25:YB:61:G:H8 | 1.83 | 0.43 |
| 39:YU:87:GLY:O | 40:YV:50:PRO:HD3 | 2.18 | 0.43 |
| 1:QA:538:G:H2' | 1:QA:539:A:H8 | 1.83 | 0.43 |
| 1:QA:582:U:H5'' | 15:QO:68:ARG:HH22 | 1.83 | 0.43 |
| 1:QA:851:G:H2' | 1:QA:852:G:C8 | 2.53 | 0.43 |
| 4:QD:20:TYR:HD2 | 4:QD:26:CYS:HB3 | 1.83 | 0.43 |
| 8:QH:7:ALA:HB2 | 8:QH:85:ARG:HD3 | 2.00 | 0.43 |
| 9:QI:4:TYR:HB2 | 9:QI:19:LEU:HB2 | 2.00 | 0.43 |
| 17:QQ:57:VAL:HG12 | 17:QQ:76:LEU:HA | 2.01 | 0.43 |
| 54:R9:11:CYS:HB2 | 54:R9:13:LYS:HD2 | 1.99 | 0.43 |
| 24:RA:2731:G:OP1 | 27:RE:169:ASN:ND2 | 2.45 | 0.43 |
| 34:RP:97:PRO:HD3 | 34:RP:126:VAL:O | 2.18 | 0.43 |
| 39:RU:50:ARG:O | 39:RU:54:LYS:NZ | 2.47 | 0.43 |
| 1:XA:1022:G:H2' | 1:XA:1023:G:H8 | 1.83 | 0.43 |
| 1:XA:1425:U:H2' | 1:XA:1426:C:H6 | 1.83 | 0.43 |
| 1:XA:298:A:H2' | 1:XA:299:G:C8 | 2.53 | 0.43 |
| 1:XA:346:G:H1' | 1:XA:347:G:H5' | 2.01 | 0.43 |
| 1:XA:552:U:H2' | 1:XA:553:A:H8 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:806:C:H2' | 1:XA:807:A:H8 | 1.82 | 0.43 |
| 12:XL:32:PHE:HE1 | 12:XL:86:ARG:HG3 | 1.84 | 0.43 |
| 24:YA:1062:G:H1 | 24:YA:1076:C:N4 | 2.16 | 0.43 |
| 24:YA:1161:C:H2' | 24:YA:1162:G:C8 | 2.53 | 0.43 |
| 24:YA:1336:A:H2' | 24:YA:1337:G:H8 | 1.82 | 0.43 |
| 24:YA:2138:C:H2' | 24:YA:2139:C:C6 | 2.53 | 0.43 |
| 24:YA:2292:C:H2' | 24:YA:2293:C:C6 | 2.52 | 0.43 |
| 24:YA:34:C:H5' | 24:YA:35:G:OP2 | 2.18 | 0.43 |
| 24:YA:640:C:H2' | 24:YA:641:C:C6 | 2.53 | 0.43 |
| 24:YA:870:A:H2' | 24:YA:871:U:O4' | 2.18 | 0.43 |
| 29:YG:71:THR:N | 29:YG:89:GLY:O | 2.51 | 0.43 |
| 1:QA:923:A:O2' | 1:QA:1399:C:OP2 | 2.31 | 0.43 |
| 1:QA:1443:G:C6 | 38:RT:118:ARG:HB2 | 2.53 | 0.43 |
| 1:QA:269:C:H2' | 1:QA:270:A:C8 | 2.52 | 0.43 |
| 1:QA:396:G:O2' | 1:QA:398:C:OP1 | 2.26 | 0.43 |
| 1:QA:551:U:H2' | 1:QA:552:U:C6 | 2.53 | 0.43 |
| 1:QA:950:U:H2' | 1:QA:951:G:C8 | 2.53 | 0.43 |
| 3:QC:39:ILE:O | 3:QC:43:LEU:HG | 2.18 | 0.43 |
| 6:QF:82:ARG:HG3 | 6:QF:84:ASN:H | 1.83 | 0.43 |
| 8:QH:46:LYS:N | 8:QH:64:LYS:HG3 | 2.33 | 0.43 |
| 14:QN:29:ARG:HH12 | 14:QN:41:ARG:H | 1.66 | 0.43 |
| 15:QO:60:VAL:HA | 15:QO:63:ARG:HG2 | 2.00 | 0.43 |
| 17:QQ:87:LYS:HB3 | 17:QQ:87:LYS:HE3 | 1.88 | 0.43 |
| 22:QV:22:A:H61 | 22:QV:47:G:H2' | 1.82 | 0.43 |
| 46:R1:53:VAL:HG13 | 46:R1:74:VAL:HG23 | 1.99 | 0.43 |
| 24:RA:2368:C:H2' | 24:RA:2369:A:C8 | 2.51 | 0.43 |
| 24:RA:345:A:O2' | 24:RA:347:A:N7 | 2.35 | 0.43 |
| 32:RN:21:LYS:HB2 | 32:RN:26:LEU:HD12 | 2.00 | 0.43 |
| 33:RO:22:ILE:HB | 33:RO:40:VAL:HG13 | 1.99 | 0.43 |
| 36:RR:3:HIS:O | 36:RR:5:LYS:N | 2.50 | 0.43 |
| 39:RU:87:GLY:O | 40:RV:50:PRO:HD3 | 2.19 | 0.43 |
| 1:XA:992:U:O2' | 1:XA:993:G:OP2 | 2.26 | 0.43 |
| 24:YA:1193:G:H2' | 24:YA:1194:A:C8 | 2.53 | 0.43 |
| 24:YA:1267:U:H2' | 24:YA:1268:A:C8 | 2.53 | 0.43 |
| 24:YA:1400:G:H2' | 24:YA:1401:G:C8 | 2.53 | 0.43 |
| 24:YA:1550:C:H2' | 24:YA:1551:C:H6 | 1.83 | 0.43 |
| 24:YA:2115:G:N2 | 24:YA:2165:G:N7 | 2.67 | 0.43 |
| 24:YA:244:A:O2' | 34:YP:74:GLU:N | 2.47 | 0.43 |
| 24:YA:2688:U:OP1 | 24:YA:2713:A:N6 | 2.51 | 0.43 |
| 24:YA:297:C:H2' | 24:YA:298:G:O4' | 2.18 | 0.43 |
| 24:YA:468:G:H5'' | 28:YF:60:SER:HB2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:YA:547:A:H2' | 24:YA:548:A:C8 | 2.53 | 0.43 |
| 24:YA:881:G:H3' | 24:YA:882:G:H8 | 1.83 | 0.43 |
| 29:YG:145:THR:O | 29:YG:146:TYR:HB3 | 2.18 | 0.43 |
| 29:YG:34:LEU:HD12 | 29:YG:172:LEU:HD21 | 2.00 | 0.43 |
| 30:YH:102:ALA:HA | 30:YH:117:PRO:HD3 | 2.01 | 0.43 |
| 7:QG:18:TYR:CG | 7:QG:59:LEU:HD21 | 2.54 | 0.43 |
| 9:QI:91:ASP:OD2 | 9:QI:93:ARG:NH2 | 2.51 | 0.43 |
| 1:QA:1202:G:C5 | 14:QN:42:ILE:HD13 | 2.52 | 0.43 |
| 24:RA:1796:U:H2' | 24:RA:1797:C:H6 | 1.83 | 0.43 |
| 24:RA:1817:G:OP2 | 26:RD:157:ARG:NH2 | 2.51 | 0.43 |
| 24:RA:1941:C:N4 | 24:RA:1965:C:O4' | 2.52 | 0.43 |
| 24:RA:570:G:H2' | 24:RA:2030:A:C6 | 2.53 | 0.43 |
| 24:RA:2476:A:H2' | 24:RA:2477:C:C6 | 2.53 | 0.43 |
| 24:RA:270(H):C:H2' | 24:RA:270(I):G:C8 | 2.54 | 0.43 |
| 44:RZ:149:SER:OG | 44:RZ:150:LEU:N | 2.50 | 0.43 |
| 44:RZ:182:LYS:O | 44:RZ:182:LYS:NZ | 2.42 | 0.43 |
| 1:XA:1013:G:N2 | 1:XA:1015:A:H3' | 2.34 | 0.43 |
| 1:XA:1407:C:H2' | 1:XA:1408:A:H8 | 1.83 | 0.43 |
| 1:XA:266:G:H5' | 1:XA:268:C:H5 | 1.82 | 0.43 |
| 1:XA:339:C:H2' | 1:XA:340:U:C6 | 2.54 | 0.43 |
| 2:XB:35:GLU:OE1 | 2:XB:36:ARG:N | 2.51 | 0.43 |
| 4:XD:165:MET:HA | 4:XD:168:ARG:HD3 | 2.00 | 0.43 |
| 4:XD:20:TYR:O | 4:XD:20:TYR:CD1 | 2.71 | 0.43 |
| 4:XD:75:PHE:HE1 | 4:XD:97:LEU:HD21 | 1.83 | 0.43 |
| 15:XO:29:VAL:HG21 | 15:XO:81:LEU:HD21 | 2.00 | 0.43 |
| 22:XV:1:C:H2' | 22:XV:2:G:C8 | 2.54 | 0.43 |
| 48:Y3:2:PRO:HG2 | 48:Y3:39:ASP:HB3 | 1.99 | 0.43 |
| 24:YA:1429:G:H2' | 24:YA:1430:C:C6 | 2.52 | 0.43 |
| 24:YA:1680:U:H2' | 24:YA:1681:G:O4' | 2.18 | 0.43 |
| 24:YA:1825:A:H2' | 24:YA:1826:G:H8 | 1.83 | 0.43 |
| 24:YA:2340:G:H2' | 24:YA:2341:G:C8 | 2.54 | 0.43 |
| 26:YD:142:VAL:HG13 | 26:YD:193:VAL:HA | 2.00 | 0.43 |
| 28:YF:40:GLN:HE22 | 28:YF:182:ASN:HB2 | 1.83 | 0.43 |
| 24:YA:2377:A:H4' | 37:YS:111:GLU:O | 2.18 | 0.43 |
| 1:QA:191(E):G:H2' | 1:QA:191(F):U:C6 | 2.54 | 0.43 |
| 1:QA:327:A:O2' | 1:QA:328:C:O4' | 2.32 | 0.43 |
| 1:QA:628:G:H2' | 1:QA:629:G:H8 | 1.82 | 0.43 |
| 1:QA:824:C:H2' | 1:QA:825:G:H8 | 1.84 | 0.43 |
| 24:RA:1357:U:H2' | 24:RA:1358:G:O4' | 2.19 | 0.43 |
| 24:RA:1478:G:H2' | 24:RA:1479:G:H8 | 1.83 | 0.43 |
| 24:RA:2566:A:H4' | 24:RA:2567:G:O5' | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 24:RA:2728:U:H2' | 24:RA:2729:G:C8 | 2.53 | 0.43 |
| 24:RA:476:G:N1 | 24:RA:479:A:OP2 | 2.51 | 0.43 |
| 24:RA:819:A:OP2 | 24:RA:1187:G:N2 | 2.48 | 0.43 |
| 41:RW:33:ARG:NE | 41:RW:52:GLU:OE2 | 2.52 | 0.43 |
| 44:RZ:45:ASP:OD1 | 44:RZ:49:ARG:NE | 2.51 | 0.43 |
| 1:XA:1190:G:H3' | 3:XC:3:ASN:ND2 | 2.34 | 0.43 |
| 1:XA:1502:A:H2 | 1:XA:1505:G:H1 | 1.66 | 0.43 |
| 1:XA:304:U:H2' | 1:XA:305:G:C8 | 2.54 | 0.43 |
| 1:XA:514:C:H2' | 1:XA:515:G:C8 | 2.50 | 0.43 |
| 1:XA:703:G:H4' | 1:XA:704:A:O5' | 2.19 | 0.43 |
| 1:XA:619:U:N3 | 4:XD:134:ASP:OD1 | 2.36 | 0.43 |
| 8:XH:14:ARG:HB2 | 8:XH:83:ILE:HD11 | 2.00 | 0.43 |
| 13:XM:97:PRO:HG3 | 13:XM:110:ARG:HB3 | 2.00 | 0.43 |
| 53:Y8:29:LYS:HB2 | 53:Y8:33:ASN:HD21 | 1.84 | 0.43 |
| 24:YA:1546:C:H5' | 24:YA:1547:C:H5' | 2.00 | 0.43 |
| 24:YA:24:G:H1' | 41:YW:77:ASP:HB3 | 2.00 | 0.43 |
| 24:YA:2543:G:H2' | 24:YA:2544:G:C8 | 2.54 | 0.43 |
| 24:YA:2777:G:OP2 | 24:YA:2781:A:O2' | 2.36 | 0.43 |
| 24:YA:394:A:H2' | 24:YA:395:U:O4' | 2.18 | 0.43 |
| 25:YB:3:C:H2' | 25:YB:4:C:H6 | 1.83 | 0.43 |
| 34:YP:90:ARG:HG3 | 34:YP:91:PHE:CD1 | 2.54 | 0.43 |
| 24:YA:870:A:P | 35:YQ:6:ARG:HH21 | 2.41 | 0.43 |
| 1:QA:412:A:H4' | 1:QA:413:G:O5' | 2.18 | 0.43 |
| 7:QG:45:ASP:O | 7:QG:49:ILE:HG12 | 2.19 | 0.43 |
| 7:QG:74:GLU:O | 7:QG:76:ARG:NH1 | 2.51 | 0.43 |
| 8:QH:99:GLU:N | 8:QH:99:GLU:OE2 | 2.51 | 0.43 |
| 1:QA:277:C:H5' | 17:QQ:68:ARG:HH22 | 1.84 | 0.43 |
| 24:RA:2271:G:OP1 | 45:R0:18:ALA:HB1 | 2.18 | 0.43 |
| 24:RA:1035:U:H2' | 24:RA:1036:G:H8 | 1.83 | 0.43 |
| 24:RA:1124:C:H2' | 24:RA:1125:G:O4' | 2.18 | 0.43 |
| 24:RA:144:C:H2' | 24:RA:145:G:H8 | 1.83 | 0.43 |
| 24:RA:1853:A:H2' | 24:RA:1854:A:H8 | 1.84 | 0.43 |
| 24:RA:186:G:H2' | 24:RA:187:G:C8 | 2.54 | 0.43 |
| 24:RA:2018:G:H2' | 24:RA:2019:A:C8 | 2.53 | 0.43 |
| 24:RA:2784:C:H2' | 24:RA:2785:C:H6 | 1.84 | 0.43 |
| 24:RA:730:C:H2' | 24:RA:731:C:H6 | 1.84 | 0.43 |
| 24:RA:807:U:H2' | 24:RA:808:G:H8 | 1.83 | 0.43 |
| 33:RO:68:GLU:HG3 | 33:RO:78:ARG:HD3 | 2.01 | 0.43 |
| 36:RR:12:ARG:O | 36:RR:17:ARG:NH2 | 2.52 | 0.43 |
| 1:XA:115:G:C6 | 1:XA:313:A:N1 | 2.86 | 0.43 |
| 1:XA:401:C:H2' | 1:XA:402:G:H8 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:407:G:H5'' | 4:XD:115:ARG:HB3 | 2.01 | 0.43 |
| 1:XA:939:G:H2' | 1:XA:940:C:C6 | 2.53 | 0.43 |
| 5:XE:39:GLY:HA2 | 5:XE:69:VAL:HB | 2.00 | 0.43 |
| 8:XH:21:LYS:O | 8:XH:65:TYR:OH | 2.25 | 0.43 |
| 10:XJ:78:ASN:HB2 | 10:XJ:81:THR:HG23 | 2.01 | 0.43 |
| 24:YA:1035:U:H2' | 24:YA:1036:G:C8 | 2.54 | 0.43 |
| 24:YA:1796:U:H2' | 24:YA:1797:C:H6 | 1.82 | 0.43 |
| 24:YA:2356:C:H2' | 24:YA:2357:U:O4' | 2.19 | 0.43 |
| 24:YA:2443:C:H2' | 24:YA:2444:G:C8 | 2.52 | 0.43 |
| 24:YA:264:C:H2' | 24:YA:265:A:H5'' | 2.00 | 0.43 |
| 24:YA:519:U:H2' | 24:YA:520:G:C8 | 2.54 | 0.43 |
| 24:YA:839:U:H2' | 24:YA:840:C:C6 | 2.54 | 0.43 |
| 39:YU:62:ILE:HD11 | 39:YU:93:LYS:HD3 | 2.01 | 0.43 |
| 41:YW:110:LYS:HG3 | 41:YW:111:HIS:CD2 | 2.54 | 0.43 |
| 44:YZ:158:PRO:HD2 | 44:YZ:161:VAL:HB | 2.00 | 0.43 |
| 44:YZ:14:LYS:HA | 44:YZ:15:PRO:HD3 | 1.86 | 0.43 |
| 1:QA:345:C:H3' | 38:RT:41:ARG:NH1 | 2.32 | 0.43 |
| 1:QA:745:C:H5'' | 1:QA:851:G:H1' | 2.00 | 0.43 |
| 3:QC:18:TRP:O | 3:QC:54:ARG:NH2 | 2.50 | 0.43 |
| 15:QO:24:SER:OG | 15:QO:25:THR:N | 2.50 | 0.43 |
| 22:QV:36:G:H2' | 22:QV:37:G:C8 | 2.53 | 0.43 |
| 24:RA:1230:C:H2' | 24:RA:1231:G:C8 | 2.53 | 0.43 |
| 24:RA:1536:A:H5'' | 24:RA:1537:C:C6 | 2.54 | 0.43 |
| 24:RA:2148:G:H2' | 24:RA:2149:G:H8 | 1.84 | 0.43 |
| 24:RA:2344:U:OP1 | 51:R6:37:ARG:HD3 | 2.19 | 0.43 |
| 24:RA:2648:C:H2' | 24:RA:2649:U:C6 | 2.53 | 0.43 |
| 24:RA:263:C:H2' | 24:RA:264:C:O4' | 2.18 | 0.43 |
| 25:RB:15:A:H5' | 25:RB:16:G:C8 | 2.53 | 0.43 |
| 27:RE:24:THR:OG1 | 27:RE:186:GLY:HA2 | 2.19 | 0.43 |
| 32:RN:18:ALA:HA | 32:RN:26:LEU:HD11 | 2.01 | 0.43 |
| 35:RQ:18:LYS:HE3 | 35:RQ:18:LYS:HB3 | 1.91 | 0.43 |
| 35:RQ:21:THR:HB | 35:RQ:22:LYS:H | 1.62 | 0.43 |
| 36:RR:45:ARG:HA | 36:RR:95:THR:HG21 | 1.99 | 0.43 |
| 1:XA:1079:G:H2' | 1:XA:1080:A:C8 | 2.54 | 0.43 |
| 1:XA:244:U:H4' | 1:XA:245:C:O5' | 2.19 | 0.43 |
| 1:XA:505:G:H2' | 1:XA:506:G:H8 | 1.84 | 0.43 |
| 1:XA:674:G:H2' | 1:XA:675:A:C8 | 2.43 | 0.43 |
| 1:XA:750:G:N3 | 15:XO:23:GLY:HA3 | 2.34 | 0.43 |
| 1:XA:87:A:H2' | 1:XA:88:C:C6 | 2.52 | 0.43 |
| 4:XD:11:LEU:HD13 | 4:XD:66:ARG:HG2 | 2.00 | 0.43 |
| 8:XH:85:ARG:HA | 8:XH:135:CYS:HB2 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:YA:1062:G:N2 | 24:YA:1078:U:H1' | 2.32 | 0.43 |
| 24:YA:1246:A:OP1 | 34:YP:15:ARG:NH2 | 2.40 | 0.43 |
| 24:YA:1278:A:H2' | 24:YA:1279:G:H8 | 1.84 | 0.43 |
| 24:YA:184:C:O2' | 24:YA:217:G:N3 | 2.49 | 0.43 |
| 24:YA:20:C:H2' | 24:YA:21:A:H8 | 1.82 | 0.43 |
| 25:YB:86:G:H2' | 25:YB:87:G:H8 | 1.82 | 0.43 |
| 1:QA:1244:C:H2' | 1:QA:1245:A:C8 | 2.54 | 0.43 |
| 1:QA:298:A:C8 | 1:QA:298:A:OP1 | 2.70 | 0.43 |
| 2:QB:121:LEU:O | 2:QB:124:SER:OG | 2.37 | 0.43 |
| 4:QD:165:MET:HA | 4:QD:168:ARG:HD3 | 2.00 | 0.43 |
| 1:QA:19:C:OP1 | 5:QE:127:ASN:HB2 | 2.18 | 0.43 |
| 12:QL:32:PHE:HE2 | 12:QL:86:ARG:HG3 | 1.82 | 0.43 |
| 13:QM:3:ARG:HG3 | 49:R4:34:GLU:HB3 | 2.01 | 0.43 |
| 24:RA:1751:C:H2' | 24:RA:1752:C:C6 | 2.54 | 0.43 |
| 24:RA:1638:C:C5' | 24:RA:2710:C:O2' | 2.63 | 0.43 |
| 24:RA:2868:A:H2' | 24:RA:2869:G:C8 | 2.54 | 0.43 |
| 24:RA:675:A:C8 | 24:RA:804:A:C6 | 3.06 | 0.43 |
| 26:RD:9:TYR:CD2 | 26:RD:10:THR:HG23 | 2.53 | 0.43 |
| 24:RA:1657:C:O2' | 27:RE:133:LYS:HG2 | 2.19 | 0.43 |
| 24:RA:2635:C:H5'' | 27:RE:78:LEU:HA | 1.99 | 0.43 |
| 32:RN:30:ILE:HG23 | 32:RN:52:VAL:HG11 | 2.01 | 0.43 |
| 1:XA:119:A:N7 | 1:XA:288:A:C6 | 2.87 | 0.43 |
| 1:XA:269:C:H2' | 1:XA:270:A:C8 | 2.53 | 0.43 |
| 1:XA:345:C:H4' | 1:XA:346:G:O5' | 2.18 | 0.43 |
| 1:XA:413:G:OP2 | 1:XA:413:G:H8 | 2.02 | 0.43 |
| 1:XA:582:U:H2' | 1:XA:583:A:C8 | 2.53 | 0.43 |
| 1:XA:639:G:H2' | 1:XA:640:A:H8 | 1.83 | 0.43 |
| 10:XJ:53:PRO:HG2 | 10:XJ:54:PHE:CE2 | 2.53 | 0.43 |
| 10:XJ:8:LEU:HB2 | 10:XJ:70:ARG:HB2 | 2.00 | 0.43 |
| 13:XM:82:MET:HG2 | 13:XM:93:ARG:HG2 | 2.00 | 0.43 |
| 48:Y3:37:LEU:HA | 48:Y3:37:LEU:HD13 | 1.77 | 0.43 |
| 24:YA:1505:C:H2' | 24:YA:1506:C:C6 | 2.53 | 0.43 |
| 24:YA:37:C:H2' | 24:YA:38:A:H8 | 1.84 | 0.43 |
| 24:YA:680:G:H2' | 24:YA:681:G:H8 | 1.84 | 0.43 |
| 26:YD:245:PRO:HA | 26:YD:246:PRO:HD3 | 1.86 | 0.43 |
| 38:YT:24:PRO:HA | 38:YT:49:VAL:HG13 | 2.01 | 0.43 |
| 1:QA:1481:U:H2' | 1:QA:1482:G:H8 | 1.83 | 0.43 |
| 1:QA:318:G:H2' | 1:QA:319:G:C8 | 2.54 | 0.43 |
| 1:QA:430:A:P | 4:QD:8:VAL:H | 2.42 | 0.43 |
| 1:QA:708:C:OP1 | 11:QK:85:ARG:NH2 | 2.43 | 0.43 |
| 3:QC:109:PRO:O | 3:QC:112:SER:OG | 2.31 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:QC:59:ARG:HA | 3:QC:63:ASN:O | 2.19 | 0.43 |
| 10:QJ:40:LEU:HD13 | 10:QJ:69:ASN:HB3 | 2.01 | 0.43 |
| 16:QP:74:LEU:HD12 | 16:QP:79:VAL:HG21 | 2.01 | 0.43 |
| 17:QQ:66:SER:O | 17:QQ:70:ARG:NH1 | 2.52 | 0.43 |
| 24:RA:839:U:H1' | 24:RA:1191:G:H1' | 2.01 | 0.43 |
| 24:RA:1790:C:H5'' | 24:RA:1791:A:OP1 | 2.18 | 0.43 |
| 24:RA:2478:A:H5' | 54:R9:31:LYS:HG2 | 2.00 | 0.43 |
| 24:RA:992:C:OP1 | 39:RU:47:TYR:OH | 2.28 | 0.43 |
| 26:RD:44:ASN:HB2 | 26:RD:48:ARG:O | 2.18 | 0.43 |
| 24:RA:2314:C:H5' | 29:RG:38:VAL:HG11 | 2.01 | 0.43 |
| 24:RA:1666:G:O2' | 33:RO:6:THR:OG1 | 2.28 | 0.43 |
| 36:RR:97:VAL:HA | 36:RR:113:LEU:O | 2.19 | 0.43 |
| 40:RV:22:VAL:HG22 | 40:RV:23:GLU:H | 1.84 | 0.43 |
| 44:RZ:48:PHE:HA | 44:RZ:51:ALA:HB3 | 2.00 | 0.43 |
| 1:XA:1022:G:H2' | 1:XA:1023:G:C8 | 2.53 | 0.43 |
| 1:XA:1250:A:H2 | 1:XA:1370:G:H1' | 1.84 | 0.43 |
| 1:XA:636:U:H2' | 1:XA:637:G:H8 | 1.83 | 0.43 |
| 1:XA:701:C:OP1 | 1:XA:702:A:O2' | 2.23 | 0.43 |
| 4:XD:14:ARG:HD2 | 4:XD:40:PRO:HD2 | 2.00 | 0.43 |
| 8:XH:13:ILE:O | 8:XH:17:THR:HG23 | 2.18 | 0.43 |
| 8:XH:77:GLU:OE2 | 8:XH:81:HIS:NE2 | 2.47 | 0.43 |
| 16:XP:12:LYS:HB3 | 16:XP:12:LYS:HE3 | 1.90 | 0.43 |
| 16:XP:68:ASP:OD1 | 16:XP:69:THR:N | 2.52 | 0.43 |
| 45:Y0:21:LEU:HD11 | 45:Y0:41:ARG:HE | 1.83 | 0.43 |
| 24:YA:1435:G:H2' | 24:YA:1436:G:C8 | 2.54 | 0.43 |
| 24:YA:20:C:H2' | 24:YA:21:A:C8 | 2.54 | 0.43 |
| 24:YA:325:G:H2' | 24:YA:326:G:H8 | 1.84 | 0.43 |
| 34:YP:88:LEU:HD12 | 34:YP:95:VAL:HG21 | 2.00 | 0.43 |
| 39:YU:106:PHE:O | 39:YU:110:VAL:HG23 | 2.19 | 0.43 |
| 1:QA:1095:U:P | 1:QA:1108:G:H1 | 2.41 | 0.43 |
| 1:QA:1224:G:H1 | 1:QA:1362(A):C:H42 | 1.66 | 0.43 |
| 1:QA:1516:G:N2 | 1:QA:1519:A:OP2 | 2.50 | 0.43 |
| 19:QS:32:LYS:HD3 | 19:QS:50:ALA:HB3 | 2.00 | 0.43 |
| 25:RB:83:G:H4' | 48:R3:52:HIS:CG | 2.54 | 0.43 |
| 24:RA:1771:C:H2' | 24:RA:1772:G:H8 | 1.84 | 0.43 |
| 24:RA:305:U:H2' | 24:RA:306:U:C6 | 2.54 | 0.43 |
| 24:RA:674:G:O2' | 28:RF:67:GLN:NE2 | 2.46 | 0.43 |
| 35:RQ:32:TYR:CE1 | 35:RQ:133:ARG:HG3 | 2.54 | 0.43 |
| 38:RT:117:ASP:O | 38:RT:121:ILE:HG12 | 2.19 | 0.43 |
| 1:XA:126:G:OP1 | 1:XA:605:U:O2' | 2.27 | 0.43 |
| 1:XA:1287:A:C2 | 1:XA:1353:G:H1' | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:45:U:H3 | 1:XA:396:G:H1 | 1.66 | 0.43 |
| 1:XA:857:C:H2' | 1:XA:858:G:O4' | 2.19 | 0.43 |
| 15:XO:15:PHE:CE1 | 15:XO:84:LYS:HD3 | 2.54 | 0.43 |
| 22:XV:64:U:H2' | 22:XV:65:C:C6 | 2.54 | 0.43 |
| 49:Y4:10:VAL:HG21 | 49:Y4:29:PRO:HG3 | 2.01 | 0.43 |
| 49:Y4:14:ILE:HB | 49:Y4:22:ILE:HB | 2.00 | 0.43 |
| 24:YA:1164:G:H2' | 24:YA:1165:U:C6 | 2.54 | 0.43 |
| 24:YA:1400:G:H2' | 24:YA:1401:G:H8 | 1.83 | 0.43 |
| 24:YA:2701:C:C3' | 24:YA:2702:U:H5'' | 2.39 | 0.43 |
| 1:QA:1126:U:H5 | 1:QA:1127:G:C4 | 2.37 | 0.42 |
| 1:QA:1400:C:N3 | 22:QV:35:C:O2 | 2.53 | 0.42 |
| 1:QA:410:G:N2 | 1:QA:432:A:H62 | 2.17 | 0.42 |
| 1:QA:768:A:H5' | 1:QA:1524:C:H1' | 2.00 | 0.42 |
| 3:QC:79:ARG:NH2 | 3:QC:82:GLU:HG2 | 2.34 | 0.42 |
| 47:R2:14:ARG:NH1 | 47:R2:66:GLU:OE1 | 2.51 | 0.42 |
| 49:R4:24:THR:OG1 | 49:R4:25:TYR:N | 2.52 | 0.42 |
| 24:RA:1210:A:H5' | 24:RA:1211:U:H2' | 2.01 | 0.42 |
| 24:RA:1411:C:N4 | 24:RA:1591:G:H1 | 2.15 | 0.42 |
| 24:RA:1657:C:H2' | 24:RA:1658:C:H6 | 1.84 | 0.42 |
| 24:RA:2637:U:H5'' | 27:RE:82:ARG:NH1 | 2.34 | 0.42 |
| 24:RA:2812:G:H2' | 24:RA:2813:A:H8 | 1.83 | 0.42 |
| 24:RA:303:U:H2' | 24:RA:304:G:C8 | 2.53 | 0.42 |
| 24:RA:307:G:N2 | 24:RA:310:A:OP2 | 2.52 | 0.42 |
| 24:RA:637:A:H4' | 24:RA:638:G:O5' | 2.19 | 0.42 |
| 24:RA:689:A:H2' | 24:RA:690:G:H8 | 1.84 | 0.42 |
| 24:RA:924:C:H2' | 24:RA:925:C:C6 | 2.54 | 0.42 |
| 40:RV:16:PRO:HD3 | 40:RV:99:ILE:HD11 | 2.01 | 0.42 |
| 40:RV:62:LEU:HB3 | 40:RV:93:GLU:HG2 | 2.00 | 0.42 |
| 1:XA:19:C:H2' | 1:XA:20:U:C6 | 2.54 | 0.42 |
| 1:XA:22:G:H4' | 1:XA:885:G:C8 | 2.54 | 0.42 |
| 1:XA:489:C:H2' | 1:XA:490:G:C8 | 2.53 | 0.42 |
| 12:XL:67:THR:OG1 | 12:XL:95:GLY:O | 2.34 | 0.42 |
| 13:XM:70:LEU:HA | 13:XM:73:GLU:HG2 | 2.00 | 0.42 |
| 24:YA:1595:G:H2' | 24:YA:1596:A:C8 | 2.53 | 0.42 |
| 24:YA:1844:C:H2' | 24:YA:1845:G:H8 | 1.84 | 0.42 |
| 24:YA:2065:C:H2' | 24:YA:2066:C:H6 | 1.83 | 0.42 |
| 24:YA:2470:G:OP1 | 35:YQ:56:ARG:NH2 | 2.52 | 0.42 |
| 29:YG:32:PRO:HB3 | 29:YG:163:ALA:HB2 | 2.01 | 0.42 |
| 29:YG:52:ILE:HD12 | 29:YG:55:LYS:HB3 | 2.01 | 0.42 |
| 30:YH:54:ARG:HD3 | 30:YH:65:HIS:HD1 | 1.82 | 0.42 |
| 36:YR:2:ARG:HB3 | 36:YR:5:LYS:HE3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:YU:39:LEU:HA | 39:YU:39:LEU:HD23 | 1.89 | 0.42 |
| 1:QA:1071:C:H2' | 1:QA:1072:G:C8 | 2.52 | 0.42 |
| 1:QA:1301:U:O2 | 1:QA:1301:U:H2' | 2.18 | 0.42 |
| 1:QA:315:A:H5'' | 1:QA:317:G:OP2 | 2.19 | 0.42 |
| 1:QA:41:G:H2' | 1:QA:42:G:C8 | 2.52 | 0.42 |
| 1:QA:452:A:H2' | 1:QA:453:A:H8 | 1.83 | 0.42 |
| 1:QA:876:G:O5' | 8:QH:14:ARG:NH1 | 2.52 | 0.42 |
| 12:QL:111:LYS:HG2 | 12:QL:111:LYS:H | 1.68 | 0.42 |
| 13:QM:56:LEU:O | 13:QM:60:VAL:HG22 | 2.20 | 0.42 |
| 22:QV:20:G:H5' | 22:QV:21:U:C5 | 2.54 | 0.42 |
| 48:R3:12:PRO:HB2 | 48:R3:20:LYS:HG2 | 2.01 | 0.42 |
| 24:RA:1297:C:H2' | 24:RA:1298:C:C6 | 2.54 | 0.42 |
| 24:RA:1401:G:H2' | 24:RA:1402:C:C6 | 2.54 | 0.42 |
| 24:RA:356:G:H2' | 24:RA:357:A:C8 | 2.55 | 0.42 |
| 28:RF:65:TRP:NE1 | 28:RF:73:ALA:O | 2.48 | 0.42 |
| 31:RI:122:GLU:OE1 | 31:RI:126:TYR:OH | 2.37 | 0.42 |
| 31:RI:33:ARG:HB2 | 31:RI:35:LEU:HD22 | 2.01 | 0.42 |
| 24:RA:2404:C:H1' | 34:RP:67:MET:HE1 | 2.01 | 0.42 |
| 44:RZ:145:GLU:HG3 | 44:RZ:146:ILE:H | 1.83 | 0.42 |
| 1:XA:17:U:H2' | 1:XA:18:C:H6 | 1.83 | 0.42 |
| 1:XA:328:C:H1' | 1:XA:329:A:OP2 | 2.19 | 0.42 |
| 1:XA:337:C:H2' | 1:XA:338:A:C8 | 2.54 | 0.42 |
| 1:XA:411:A:H62 | 1:XA:413:G:H21 | 1.67 | 0.42 |
| 1:XA:560:U:H4' | 1:XA:561:U:H5'' | 2.01 | 0.42 |
| 2:XB:84:GLU:OE1 | 2:XB:87:ARG:NH2 | 2.43 | 0.42 |
| 7:XG:115:ARG:HB2 | 7:XG:118:VAL:HG12 | 2.01 | 0.42 |
| 47:Y2:16:LEU:HD22 | 47:Y2:21:LEU:HD13 | 2.01 | 0.42 |
| 48:Y3:4:LEU:HD12 | 48:Y3:39:ASP:HB2 | 2.01 | 0.42 |
| 24:YA:1309:G:H4' | 52:Y7:7:PRO:HB2 | 2.01 | 0.42 |
| 24:YA:138:G:H22 | 42:YX:44:GLU:CD | 2.23 | 0.42 |
| 24:YA:1430:C:H2' | 24:YA:1431:U:C6 | 2.54 | 0.42 |
| 24:YA:1693:U:O2 | 26:YD:14:ARG:NH1 | 2.53 | 0.42 |
| 24:YA:1771:C:O2' | 24:YA:1786:A:O4' | 2.35 | 0.42 |
| 24:YA:1790:C:H5'' | 24:YA:1791:A:OP1 | 2.18 | 0.42 |
| 24:YA:2185:C:H2' | 24:YA:2186:G:H8 | 1.83 | 0.42 |
| 24:YA:242:G:H4' | 24:YA:243:U:O5' | 2.19 | 0.42 |
| 24:YA:278:A:O2' | 24:YA:279:C:O4' | 2.33 | 0.42 |
| 24:YA:338:G:OP1 | 43:YY:4:LYS:NZ | 2.52 | 0.42 |
| 24:YA:863:A:H2' | 24:YA:864:G:C8 | 2.54 | 0.42 |
| 26:YD:31:LYS:HD3 | 26:YD:31:LYS:HA | 1.85 | 0.42 |
| 27:YE:143:ASN:HB2 | 27:YE:147:PRO:HD2 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:YF:198:ALA:HA | 28:YF:201:VAL:HG12 | 2.02 | 0.42 |
| 44:YZ:30:ASN:OD1 | 44:YZ:33:LEU:N | 2.51 | 0.42 |
| 1:QA:1427:U:H2' | 1:QA:1428:A:C8 | 2.53 | 0.42 |
| 1:QA:806:C:H2' | 1:QA:807:A:C8 | 2.48 | 0.42 |
| 24:RA:1165:U:H2' | 24:RA:1166:C:H6 | 1.84 | 0.42 |
| 24:RA:1332:G:H8 | 24:RA:1332:G:H2' | 1.65 | 0.42 |
| 24:RA:1468:C:H2' | 24:RA:1469:A:C8 | 2.53 | 0.42 |
| 24:RA:2123:G:H2' | 24:RA:2124:G:H8 | 1.83 | 0.42 |
| 24:RA:2133:G:H1' | 24:RA:2158:A:N6 | 2.34 | 0.42 |
| 24:RA:2695:C:H2' | 24:RA:2696:U:C6 | 2.55 | 0.42 |
| 24:RA:532:A:H4' | 24:RA:533:G:C8 | 2.54 | 0.42 |
| 24:RA:689:A:H2' | 24:RA:690:G:C8 | 2.55 | 0.42 |
| 25:RB:8:U:H3 | 25:RB:112:G:H1 | 1.66 | 0.42 |
| 26:RD:50:THR:OG1 | 26:RD:51:VAL:N | 2.51 | 0.42 |
| 1:XA:166:G:H2' | 1:XA:167:G:H8 | 1.84 | 0.42 |
| 1:XA:347:G:O2' | 1:XA:348:G:H5'' | 2.19 | 0.42 |
| 1:XA:575:G:O2' | 1:XA:821:G:H5' | 2.19 | 0.42 |
| 8:XH:59:LEU:HA | 8:XH:59:LEU:HD13 | 1.81 | 0.42 |
| 9:XI:112:LYS:HA | 9:XI:119:ALA:HB2 | 2.01 | 0.42 |
| 24:YA:1670:C:H5' | 24:YA:1671:U:OP2 | 2.19 | 0.42 |
| 24:YA:2119:A:H61 | 24:YA:2168:G:N2 | 2.18 | 0.42 |
| 24:YA:521:G:H2' | 24:YA:522:G:C8 | 2.53 | 0.42 |
| 24:YA:875:G:H2' | 24:YA:876:C:C6 | 2.54 | 0.42 |
| 24:YA:882:G:H2' | 24:YA:883:G:C8 | 2.54 | 0.42 |
| 29:YG:37:VAL:HG13 | 29:YG:159:VAL:HG12 | 2.00 | 0.42 |
| 29:YG:47:LYS:HB3 | 29:YG:81:LYS:HD2 | 2.02 | 0.42 |
| 33:YO:73:ASP:OD1 | 33:YO:75:SER:OG | 2.32 | 0.42 |
| 35:YQ:32:TYR:CE1 | 35:YQ:133:ARG:HG3 | 2.54 | 0.42 |
| 44:YZ:70:LEU:HB2 | 44:YZ:91:LEU:HD21 | 2.01 | 0.42 |
| 1:QA:1286:A:H2' | 1:QA:1287:A:H4' | 2.01 | 0.42 |
| 1:QA:165:C:H2' | 1:QA:166:G:C8 | 2.51 | 0.42 |
| 1:QA:192:U:H2' | 1:QA:193:C:H6 | 1.83 | 0.42 |
| 1:QA:255:G:H2' | 1:QA:256:U:C6 | 2.54 | 0.42 |
| 1:QA:645:C:H2' | 1:QA:646:U:C6 | 2.55 | 0.42 |
| 1:QA:686:U:H1' | 11:QK:42:TRP:NE1 | 2.34 | 0.42 |
| 8:QH:34:GLU:HB3 | 8:QH:118:VAL:HG11 | 2.02 | 0.42 |
| 24:RA:1499:C:H2' | 24:RA:1500:G:H8 | 1.83 | 0.42 |
| 24:RA:2573:C:OP1 | 24:RA:2574:G:OP1 | 2.37 | 0.42 |
| 24:RA:270(V):G:H2' | 24:RA:270(W):G:H8 | 1.84 | 0.42 |
| 24:RA:96:G:H4' | 47:R2:48:HIS:CD2 | 2.54 | 0.42 |
| 35:RQ:67:ARG:O | 35:RQ:101:ARG:NH2 | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:RY:82:PRO:O | 43:RY:101:LYS:NZ | 2.50 | 0.42 |
| 1:XA:62:U:H3 | 1:XA:105:G:H1 | 1.67 | 0.42 |
| 1:XA:1244:C:H2' | 1:XA:1245:A:H8 | 1.84 | 0.42 |
| 4:XD:20:TYR:HA | 4:XD:26:CYS:SG | 2.59 | 0.42 |
| 5:XE:78:HIS:HB3 | 8:XH:107:LEU:HD22 | 2.00 | 0.42 |
| 1:XA:598:U:H4' | 8:XH:94:TYR:CG | 2.53 | 0.42 |
| 18:XR:44:LEU:HA | 18:XR:44:LEU:HD12 | 1.93 | 0.42 |
| 19:XS:65:ASN:O | 49:Y4:58:ARG:HD2 | 2.19 | 0.42 |
| 53:Y8:61:LEU:HD23 | 53:Y8:61:LEU:HA | 1.75 | 0.42 |
| 24:YA:1182:A:H2' | 24:YA:1183:G:C8 | 2.55 | 0.42 |
| 24:YA:1348:G:H2' | 24:YA:1349:A:H5'' | 2.01 | 0.42 |
| 24:YA:1637:A:H2' | 24:YA:1638:C:C6 | 2.54 | 0.42 |
| 24:YA:2081:C:H2' | 24:YA:2082:A:H8 | 1.84 | 0.42 |
| 24:YA:2635:C:OP1 | 27:YE:78:LEU:HD13 | 2.20 | 0.42 |
| 24:YA:263:C:H2' | 24:YA:264:C:O4' | 2.20 | 0.42 |
| 24:YA:2852:G:H2' | 24:YA:2853:C:C6 | 2.54 | 0.42 |
| 24:YA:562:U:H6 | 24:YA:562:U:H2' | 1.64 | 0.42 |
| 24:YA:448:U:C4 | 24:YA:583:G:H1' | 2.54 | 0.42 |
| 30:YH:153:LYS:HB2 | 30:YH:162:ILE:HD12 | 2.00 | 0.42 |
| 32:YN:47:ALA:O | 32:YN:119:ARG:NH1 | 2.52 | 0.42 |
| 33:YO:19:ILE:HG22 | 33:YO:43:VAL:HG12 | 2.01 | 0.42 |
| 39:YU:90:VAL:HG11 | 40:YV:40:LEU:HG | 2.02 | 0.42 |
| 2:QB:60:ASP:HB3 | 2:QB:64:ARG:HH12 | 1.85 | 0.42 |
| 24:RA:1161:C:H2' | 24:RA:1162:G:C8 | 2.53 | 0.42 |
| 24:RA:1336:A:H2' | 24:RA:1337:G:H8 | 1.84 | 0.42 |
| 24:RA:180:G:OP1 | 52:R7:32:LYS:HG3 | 2.20 | 0.42 |
| 24:RA:2597:G:H2' | 24:RA:2598:A:C8 | 2.54 | 0.42 |
| 24:RA:519:U:H2' | 24:RA:520:G:C8 | 2.55 | 0.42 |
| 24:RA:764:A:O2' | 24:RA:765:G:H5' | 2.20 | 0.42 |
| 24:RA:863:A:H2' | 24:RA:864:G:C8 | 2.55 | 0.42 |
| 24:RA:922:U:H2' | 24:RA:923:C:H6 | 1.84 | 0.42 |
| 25:RB:44:G:H5'' | 25:RB:45:A:OP1 | 2.18 | 0.42 |
| 27:RE:46:ALA:HB1 | 27:RE:80:GLU:HB3 | 2.02 | 0.42 |
| 28:RF:157:VAL:HG11 | 28:RF:181:LEU:HD21 | 2.02 | 0.42 |
| 41:RW:76:VAL:HG22 | 41:RW:103:ILE:HA | 2.02 | 0.42 |
| 1:XA:1172:C:H2' | 1:XA:1173:G:C8 | 2.53 | 0.42 |
| 1:XA:1305:G:OP1 | 21:XU:2:GLY:HA2 | 2.18 | 0.42 |
| 1:XA:41:G:H2' | 1:XA:42:G:C8 | 2.54 | 0.42 |
| 1:XA:583:A:H2' | 1:XA:584:G:O4' | 2.20 | 0.42 |
| 1:XA:707:C:H2' | 1:XA:708:C:C6 | 2.54 | 0.42 |
| 1:XA:78:G:H3' | 1:XA:79:G:C8 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:848:C:H2' | 1:XA:849:C:H6 | 1.84 | 0.42 |
| 8:XH:121:ASP:OD1 | 8:XH:122:ARG:N | 2.50 | 0.42 |
| 24:YA:1508:A:O2' | 24:YA:1509:C:O5' | 2.37 | 0.42 |
| 24:YA:414:C:O2 | 24:YA:1864:U:O2' | 2.36 | 0.42 |
| 26:YD:95:LEU:HA | 26:YD:95:LEU:HD23 | 1.88 | 0.42 |
| 1:QA:1298:C:H4' | 1:QA:1299:A:C8 | 2.55 | 0.42 |
| 1:QA:753:A:H4' | 1:QA:754:C:O5' | 2.18 | 0.42 |
| 14:QN:9:LYS:O | 14:QN:19:ARG:NH2 | 2.52 | 0.42 |
| 23:QX:19:C:O5' | 23:QX:19:C:H6 | 2.02 | 0.42 |
| 24:RA:1405:U:H2' | 24:RA:1406:U:C6 | 2.52 | 0.42 |
| 24:RA:1923:U:H2' | 24:RA:1924:C:C6 | 2.55 | 0.42 |
| 24:RA:2327:A:N7 | 24:RA:2388:A:N6 | 2.68 | 0.42 |
| 24:RA:2404:C:H2' | 24:RA:2405:G:O4' | 2.19 | 0.42 |
| 24:RA:2790:A:H2' | 24:RA:2791:C:H5'' | 2.02 | 0.42 |
| 24:RA:709:U:H2' | 24:RA:710:G:C8 | 2.53 | 0.42 |
| 30:RH:144:VAL:O | 30:RH:148:ILE:HD12 | 2.20 | 0.42 |
| 30:RH:153:LYS:HB3 | 30:RH:161:GLY:HA2 | 2.00 | 0.42 |
| 38:RT:8:LYS:HA | 38:RT:11:GLU:OE2 | 2.19 | 0.42 |
| 38:RT:123:GLN:HB3 | 38:RT:124:ASP:H | 1.50 | 0.42 |
| 24:RA:24:G:O2' | 41:RW:78:GLU:O | 2.34 | 0.42 |
| 44:RZ:4:ARG:HG2 | 44:RZ:58:VAL:HB | 2.00 | 0.42 |
| 1:XA:191(D):U:H2' | 1:XA:191(E):G:H8 | 1.84 | 0.42 |
| 1:XA:192:U:H2' | 1:XA:193:C:C6 | 2.54 | 0.42 |
| 1:XA:281:G:OP2 | 1:XA:281:G:H8 | 2.03 | 0.42 |
| 1:XA:300:A:O2' | 1:XA:564:C:N3 | 2.43 | 0.42 |
| 3:XC:3:ASN:HB3 | 3:XC:4:LYS:HD2 | 2.01 | 0.42 |
| 4:XD:79:PHE:HZ | 4:XD:204:ILE:HG13 | 1.85 | 0.42 |
| 5:XE:32:VAL:HG11 | 5:XE:55:VAL:HG23 | 2.02 | 0.42 |
| 11:XK:19:ALA:O | 11:XK:82:VAL:HA | 2.20 | 0.42 |
| 15:XO:57:LEU:HA | 15:XO:60:VAL:HG12 | 2.01 | 0.42 |
| 18:XR:86:VAL:HG12 | 18:XR:87:ARG:HG2 | 2.02 | 0.42 |
| 20:XT:51:GLU:HA | 20:XT:54:LYS:HG2 | 2.00 | 0.42 |
| 24:YA:2112:G:O6 | 24:YA:2169:A:N6 | 2.53 | 0.42 |
| 24:YA:2676:C:H2' | 24:YA:2677:G:C8 | 2.54 | 0.42 |
| 24:YA:1818:U:H2' | 26:YD:157:ARG:HG2 | 2.02 | 0.42 |
| 32:YN:6:PRO:HG3 | 32:YN:41:ASP:HB2 | 2.01 | 0.42 |
| 41:YW:17:VAL:HG13 | 41:YW:76:VAL:HG21 | 2.01 | 0.42 |
| 1:QA:1064:G:OP2 | 1:QA:1385:G:O2' | 2.25 | 0.42 |
| 1:QA:1189:C:H5'' | 3:QC:5:ILE:HG21 | 2.02 | 0.42 |
| 1:QA:979:C:OP1 | 1:QA:1223:C:N4 | 2.52 | 0.42 |
| 1:QA:126:G:OP1 | 1:QA:605:U:O2' | 2.21 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1322:C:OP1 | 1:QA:1322:C:H6 | 2.02 | 0.42 |
| 1:QA:1524:C:H2' | 1:QA:1525:G:C8 | 2.55 | 0.42 |
| 1:QA:164:U:H2' | 1:QA:165:C:H6 | 1.84 | 0.42 |
| 1:QA:308:C:H2' | 1:QA:309:G:C8 | 2.55 | 0.42 |
| 1:QA:812:C:H6 | 1:QA:812:C:H2' | 1.71 | 0.42 |
| 2:QB:178:ARG:NH2 | 2:QB:196:LEU:O | 2.52 | 0.42 |
| 10:QJ:13:HIS:HB3 | 10:QJ:68:HIS:ND1 | 2.34 | 0.42 |
| 10:QJ:41:PRO:O | 10:QJ:43:ARG:NH1 | 2.53 | 0.42 |
| 12:QL:76:ASN:N | 12:QL:76:ASN:OD1 | 2.52 | 0.42 |
| 16:QP:67:THR:HG22 | 16:QP:68:ASP:N | 2.34 | 0.42 |
| 22:QV:2:G:H2' | 22:QV:3:G:H8 | 1.85 | 0.42 |
| 24:RA:857:C:OP1 | 45:R0:69:PHE:HD2 | 2.02 | 0.42 |
| 24:RA:1258:C:H2' | 24:RA:1259:G:C8 | 2.55 | 0.42 |
| 24:RA:1752:C:H2' | 24:RA:1753:G:C8 | 2.54 | 0.42 |
| 24:RA:2081:C:H2' | 24:RA:2082:A:C8 | 2.54 | 0.42 |
| 24:RA:2448:A:OP2 | 24:RA:2499:C:OP2 | 2.37 | 0.42 |
| 24:RA:2462:U:H2' | 24:RA:2463:C:C6 | 2.55 | 0.42 |
| 24:RA:2514:U:H2' | 24:RA:2515:C:H6 | 1.85 | 0.42 |
| 1:XA:1308:U:H2' | 1:XA:1309:G:C8 | 2.55 | 0.42 |
| 1:XA:1513:A:H2' | 1:XA:1514:C:H6 | 1.85 | 0.42 |
| 1:XA:328:C:H4' | 1:XA:329:A:O5' | 2.20 | 0.42 |
| 1:XA:784:C:H4' | 24:YA:1837:C:OP1 | 2.20 | 0.42 |
| 2:XB:185:ILE:HA | 2:XB:199:TYR:O | 2.19 | 0.42 |
| 7:XG:103:TRP:CD2 | 7:XG:137:LYS:HD3 | 2.54 | 0.42 |
| 11:XK:67:ASP:O | 11:XK:71:LYS:HG2 | 2.20 | 0.42 |
| 11:XK:86:GLY:O | 11:XK:91:ARG:NH1 | 2.50 | 0.42 |
| 13:XM:10:PRO:HG3 | 13:XM:22:ILE:HD11 | 2.00 | 0.42 |
| 16:XP:26:ARG:HD3 | 16:XP:26:ARG:HA | 1.94 | 0.42 |
| 23:XX:1:G:H2' | 23:XX:2:G:C8 | 2.53 | 0.42 |
| 24:YA:1454:U:O2' | 24:YA:1455:G:N7 | 2.41 | 0.42 |
| 24:YA:2384:G:OP2 | 45:Y0:55:ARG:NH2 | 2.52 | 0.42 |
| 24:YA:630:G:N2 | 24:YA:633:A:OP2 | 2.26 | 0.42 |
| 24:YA:813:U:H2' | 24:YA:814:C:C6 | 2.55 | 0.42 |
| 26:YD:79:VAL:HG21 | 26:YD:111:LEU:HD11 | 2.01 | 0.42 |
| 27:YE:174:ASP:HB3 | 27:YE:183:LEU:HD12 | 2.01 | 0.42 |
| 32:YN:114:ARG:HG2 | 32:YN:114:ARG:H | 1.63 | 0.42 |
| 1:QA:1218:C:H2' | 1:QA:1219:U:C6 | 2.54 | 0.42 |
| 1:QA:35:G:H2' | 1:QA:36:C:C6 | 2.55 | 0.42 |
| 1:QA:784:C:H4' | 24:RA:1837:C:OP1 | 2.20 | 0.42 |
| 24:RA:1166:C:H2' | 24:RA:1167:U:C6 | 2.55 | 0.42 |
| 24:RA:1191:G:P | 34:RP:18:ARG:HH22 | 2.42 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:RA:1667:G:OP2 | 24:RA:1667:G:H8 | 2.03 | 0.42 |
| 24:RA:2385:C:H2' | 24:RA:2386:C:C6 | 2.55 | 0.42 |
| 24:RA:2503:A:O2' | 24:RA:2505:G:OP2 | 2.28 | 0.42 |
| 24:RA:30:G:H2' | 24:RA:31:C:C6 | 2.55 | 0.42 |
| 24:RA:935:C:H2' | 24:RA:936:C:H6 | 1.84 | 0.42 |
| 24:RA:947:G:H2' | 24:RA:948:G:C8 | 2.55 | 0.42 |
| 26:RD:71:ASP:HB2 | 26:RD:103:ARG:HH12 | 1.84 | 0.42 |
| 30:RH:154:PRO:HG3 | 30:RH:162:ILE:HG13 | 2.01 | 0.42 |
| 32:RN:16:ILE:HG21 | 32:RN:26:LEU:HD21 | 2.00 | 0.42 |
| 34:RP:94:GLU:O | 34:RP:96:THR:HG23 | 2.19 | 0.42 |
| 38:RT:111:ARG:O | 38:RT:112:ARG:HB3 | 2.20 | 0.42 |
| 1:XA:1145:C:H4' | 1:XA:1146:A:H5' | 2.01 | 0.42 |
| 1:XA:1250:A:N3 | 1:XA:1370:G:O2' | 2.40 | 0.42 |
| 1:XA:565:U:OP2 | 1:XA:566:G:O2' | 2.19 | 0.42 |
| 1:XA:62:U:H2' | 1:XA:63:C:C6 | 2.54 | 0.42 |
| 24:YA:1057:A:N6 | 24:YA:1087:G:OP2 | 2.52 | 0.42 |
| 24:YA:1258:C:H2' | 24:YA:1259:G:C8 | 2.55 | 0.42 |
| 24:YA:1593:G:H2' | 24:YA:1594:G:H8 | 1.84 | 0.42 |
| 24:YA:1794:U:H2' | 24:YA:1795:C:C6 | 2.55 | 0.42 |
| 24:YA:210:C:H2' | 24:YA:211:A:C8 | 2.55 | 0.42 |
| 24:YA:2576:G:O2' | 24:YA:2579:C:OP2 | 2.31 | 0.42 |
| 24:YA:2593:U:H2' | 24:YA:2594:C:C6 | 2.55 | 0.42 |
| 24:YA:2657:A:H1' | 24:YA:2665:A:N6 | 2.35 | 0.42 |
| 24:YA:2880:C:O3' | 36:YR:90:ARG:NH1 | 2.52 | 0.42 |
| 24:YA:637:A:H4' | 24:YA:638:G:O5' | 2.19 | 0.42 |
| 28:YF:186:ILE:HG23 | 28:YF:192:LEU:HD12 | 2.02 | 0.42 |
| 29:YG:166:ASP:OD1 | 29:YG:166:ASP:N | 2.53 | 0.42 |
| 33:YO:22:ILE:HB | 33:YO:40:VAL:HG23 | 2.01 | 0.42 |
| 35:YQ:29:PHE:N | 35:YQ:105:GLU:OE2 | 2.34 | 0.42 |
| 1:QA:1343:G:H2' | 1:QA:1344:C:C6 | 2.55 | 0.42 |
| 1:QA:335:C:H2' | 1:QA:336:C:H6 | 1.85 | 0.42 |
| 1:QA:963:G:H21 | 10:QJ:55:LYS:HE2 | 1.85 | 0.42 |
| 12:QL:59:ARG:NH1 | 12:QL:60:LEU:O | 2.53 | 0.42 |
| 14:QN:29:ARG:HH22 | 14:QN:41:ARG:HG2 | 1.85 | 0.42 |
| 19:QS:80:TYR:HD2 | 19:QS:82:GLY:H | 1.68 | 0.42 |
| 21:QU:25:LYS:HE2 | 21:QU:25:LYS:HB2 | 1.82 | 0.42 |
| 22:QV:55:U:H2' | 22:QV:56:U:C6 | 2.54 | 0.42 |
| 24:RA:2097:C:H2' | 24:RA:2098:U:C6 | 2.55 | 0.42 |
| 24:RA:270(R):G:H2' | 24:RA:270(S):G:C8 | 2.55 | 0.42 |
| 24:RA:51:G:H8 | 24:RA:51:G:OP2 | 2.03 | 0.42 |
| 24:RA:582:G:H2' | 24:RA:583:G:C8 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:RA:660:G:H4' | 28:RF:38:ARG:NH1 | 2.35 | 0.42 |
| 24:RA:671:C:H2' | 24:RA:672:C:C6 | 2.55 | 0.42 |
| 24:RA:760:G:H2' | 24:RA:761:A:O4' | 2.19 | 0.42 |
| 24:RA:78:A:H2' | 24:RA:79:G:C8 | 2.55 | 0.42 |
| 30:RH:149:ARG:NH2 | 30:RH:167:GLU:OE2 | 2.48 | 0.42 |
| 32:RN:23:LEU:HD13 | 32:RN:60:ILE:HD12 | 2.02 | 0.42 |
| 1:XA:781:A:H4' | 1:XA:1522:U:O2' | 2.20 | 0.42 |
| 1:XA:218:C:H2' | 1:XA:219:C:C6 | 2.55 | 0.42 |
| 1:XA:261:U:H3 | 1:XA:263:A:H3' | 1.85 | 0.42 |
| 1:XA:358:U:C6 | 1:XA:358:U:C3' | 3.03 | 0.42 |
| 1:XA:359:U:H5'' | 1:XA:360:A:OP2 | 2.20 | 0.42 |
| 1:XA:382:A:H2' | 1:XA:383:A:H8 | 1.84 | 0.42 |
| 1:XA:563:A:H2' | 1:XA:567:G:C8 | 2.55 | 0.42 |
| 11:XK:22:HIS:HB3 | 11:XK:29:ILE:HG23 | 2.00 | 0.42 |
| 12:XL:77:LEU:HD21 | 12:XL:107:ALA:HB2 | 2.00 | 0.42 |
| 17:XQ:6:LEU:HA | 17:XQ:6:LEU:HD13 | 1.87 | 0.42 |
| 24:YA:1438:U:H2' | 24:YA:1439:A:C8 | 2.54 | 0.42 |
| 24:YA:1841:U:H2' | 24:YA:1842:G:H8 | 1.84 | 0.42 |
| 24:YA:315:G:H2' | 24:YA:316:C:C6 | 2.55 | 0.42 |
| 24:YA:896:A:O2' | 44:YZ:176:PRO:HG3 | 2.20 | 0.42 |
| 26:YD:25:THR:O | 26:YD:27:THR:N | 2.51 | 0.42 |
| 38:YT:124:ASP:N | 38:YT:124:ASP:OD1 | 2.49 | 0.42 |
| 1:QA:1268:A:H1' | 1:QA:1326:C:O2' | 2.20 | 0.42 |
| 1:QA:407:G:H2' | 1:QA:408:A:H8 | 1.83 | 0.42 |
| 1:QA:920:U:H2' | 1:QA:921:U:C6 | 2.55 | 0.42 |
| 12:QL:69:TYR:O | 12:QL:100:ILE:HG22 | 2.20 | 0.42 |
| 20:QT:43:LEU:HB3 | 20:QT:52:ALA:HB2 | 2.01 | 0.42 |
| 22:QV:65:C:H2' | 22:QV:66:U:C6 | 2.54 | 0.42 |
| 24:RA:1756:G:H4' | 24:RA:1758:G:O4' | 2.20 | 0.42 |
| 24:RA:20:C:H2' | 24:RA:21:A:C8 | 2.55 | 0.42 |
| 24:RA:347:A:H2' | 24:RA:348:G:H8 | 1.85 | 0.42 |
| 26:RD:39:LYS:HE2 | 26:RD:60:ARG:HB2 | 2.02 | 0.42 |
| 24:RA:1568:G:H5'' | 26:RD:61:LEU:HG | 2.01 | 0.42 |
| 27:RE:9:VAL:HB | 27:RE:25:VAL:HG23 | 2.01 | 0.42 |
| 1:XA:1121:U:H2' | 1:XA:1122:U:C6 | 2.55 | 0.42 |
| 1:XA:1352:C:H2' | 1:XA:1353:G:C8 | 2.55 | 0.42 |
| 1:XA:1496:C:H2' | 1:XA:1497:G:C8 | 2.54 | 0.42 |
| 1:XA:358:U:C6 | 1:XA:358:U:H3' | 2.55 | 0.42 |
| 1:XA:537:G:H2' | 1:XA:538:G:H8 | 1.85 | 0.42 |
| 1:XA:584:G:H2' | 1:XA:585:G:H8 | 1.85 | 0.42 |
| 5:XE:83:GLU:HG2 | 5:XE:88:LYS:HG3 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:XM:17:VAL:O | 13:XM:20:THR:OG1 | 2.22 | 0.42 |
| 22:XV:35:C:H2' | 22:XV:36:G:C8 | 2.55 | 0.42 |
| 24:YA:111:A:H4' | 47:Y2:69:ARG:NH2 | 2.34 | 0.42 |
| 24:YA:1756:G:H4' | 24:YA:1758:G:O4' | 2.19 | 0.42 |
| 24:YA:1771:C:H2' | 24:YA:1772:G:C8 | 2.55 | 0.42 |
| 24:YA:1796:U:H2' | 24:YA:1797:C:C6 | 2.55 | 0.42 |
| 24:YA:2020:A:N7 | 50:Y5:9:LYS:NZ | 2.63 | 0.42 |
| 24:YA:2487:G:H2' | 24:YA:2488:A:C8 | 2.55 | 0.42 |
| 24:YA:466:A:N3 | 24:YA:683:C:H1' | 2.35 | 0.42 |
| 24:YA:572:A:OP2 | 40:YV:78:LYS:NZ | 2.49 | 0.42 |
| 24:YA:580:C:H2' | 24:YA:581:C:C6 | 2.55 | 0.42 |
| 24:YA:841:A:H2' | 24:YA:842:G:C8 | 2.55 | 0.42 |
| 38:YT:26:ASP:HB2 | 38:YT:90:GLN:O | 2.20 | 0.42 |
| 1:QA:1244:C:H2' | 1:QA:1245:A:H8 | 1.84 | 0.41 |
| 1:QA:1391:U:H2' | 1:QA:1392:G:H8 | 1.85 | 0.41 |
| 1:QA:1500:A:OP1 | 1:QA:1505:G:OP1 | 2.38 | 0.41 |
| 1:QA:647:C:H2' | 1:QA:648:A:C8 | 2.54 | 0.41 |
| 3:QC:118:GLN:O | 3:QC:122:GLU:HG3 | 2.20 | 0.41 |
| 3:QC:36:ASP:HA | 3:QC:39:ILE:HD12 | 2.01 | 0.41 |
| 1:QA:881:G:P | 12:QL:12:ARG:HH22 | 2.43 | 0.41 |
| 18:QR:73:ALA:HB1 | 18:QR:78:LEU:HD12 | 2.02 | 0.41 |
| 24:RA:108:U:H2' | 24:RA:109:G:C8 | 2.55 | 0.41 |
| 24:RA:1467:C:C5 | 24:RA:1546:C:H2' | 2.55 | 0.41 |
| 24:RA:1812:A:H2' | 24:RA:1813:G:C8 | 2.55 | 0.41 |
| 24:RA:2467:C:OP1 | 54:R9:6:SER:OG | 2.33 | 0.41 |
| 27:RE:49:LEU:HD13 | 27:RE:49:LEU:HA | 1.90 | 0.41 |
| 30:RH:25:LYS:HZ2 | 30:RH:26:VAL:H | 1.66 | 0.41 |
| 32:RN:47:ALA:O | 32:RN:119:ARG:NH1 | 2.53 | 0.41 |
| 33:RO:19:ILE:HG22 | 33:RO:43:VAL:HA | 2.01 | 0.41 |
| 42:RX:72:LYS:NZ | 42:RX:75:ASP:OD1 | 2.39 | 0.41 |
| 1:XA:1161:C:O2' | 1:XA:1162:C:H5' | 2.20 | 0.41 |
| 1:XA:1371:G:O3' | 9:XI:69:GLY:HA3 | 2.18 | 0.41 |
| 1:XA:18:C:H5'' | 5:XE:127:ASN:HD21 | 1.84 | 0.41 |
| 1:XA:269:C:H2' | 1:XA:270:A:H8 | 1.85 | 0.41 |
| 1:XA:412:A:H4' | 1:XA:413:G:O5' | 2.19 | 0.41 |
| 1:XA:570:G:H2' | 1:XA:571:U:C6 | 2.55 | 0.41 |
| 1:XA:587:G:N2 | 1:XA:754:C:OP2 | 2.53 | 0.41 |
| 1:XA:97:U:H2' | 1:XA:99:C:H6 | 1.85 | 0.41 |
| 2:XB:76:GLN:HE22 | 2:XB:206:ASP:HB3 | 1.84 | 0.41 |
| 3:XC:132:ARG:O | 3:XC:136:GLN:HG3 | 2.20 | 0.41 |
| 7:XG:12:LEU:HD12 | 7:XG:13:GLN:H | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:1220:G:N2 | 19:XS:54:GLY:O | 2.52 | 0.41 |
| 22:XV:19:G:OP1 | 22:XV:19:G:H8 | 2.03 | 0.41 |
| 24:YA:1609:A:C6 | 24:YA:1616:A:C5 | 3.07 | 0.41 |
| 24:YA:1613:G:O2' | 52:Y7:3:ARG:NE | 2.53 | 0.41 |
| 24:YA:265:A:H61 | 24:YA:427:U:HO2' | 1.68 | 0.41 |
| 24:YA:2735:G:H2' | 24:YA:2736:G:C8 | 2.55 | 0.41 |
| 34:YP:33:ARG:HD3 | 34:YP:40:SER:HA | 2.02 | 0.41 |
| 1:QA:1064:G:HO2' | 1:QA:1065:U:P | 2.44 | 0.41 |
| 1:QA:231:G:H2' | 1:QA:232:G:H8 | 1.84 | 0.41 |
| 8:QH:53:VAL:HB | 8:QH:58:TYR:HD1 | 1.85 | 0.41 |
| 12:QL:39:VAL:HG12 | 12:QL:57:LYS:HB3 | 2.02 | 0.41 |
| 6:QF:50:TYR:CE1 | 18:QR:77:GLY:HA2 | 2.55 | 0.41 |
| 22:QV:64:U:H2' | 22:QV:65:C:C6 | 2.56 | 0.41 |
| 45:R0:38:VAL:HB | 45:R0:59:LEU:HB2 | 2.02 | 0.41 |
| 47:R2:21:LEU:HB3 | 47:R2:64:LEU:HD12 | 2.02 | 0.41 |
| 24:RA:2529:G:O6 | 54:R9:31:LYS:NZ | 2.53 | 0.41 |
| 24:RA:1114:G:H2' | 24:RA:1115:G:H8 | 1.85 | 0.41 |
| 24:RA:1164:G:H2' | 24:RA:1165:U:C6 | 2.55 | 0.41 |
| 24:RA:1173:G:H4' | 24:RA:1174:A:N7 | 2.34 | 0.41 |
| 24:RA:1314:C:OP1 | 24:RA:1332:G:OP1 | 2.38 | 0.41 |
| 24:RA:1658:C:H2' | 24:RA:1659:U:C6 | 2.55 | 0.41 |
| 24:RA:1902:C:OP1 | 26:RD:242:ARG:NH1 | 2.53 | 0.41 |
| 24:RA:38:A:H2' | 24:RA:39:C:C6 | 2.54 | 0.41 |
| 24:RA:663:G:H2' | 24:RA:664:C:C6 | 2.55 | 0.41 |
| 24:RA:78:A:H2' | 24:RA:79:G:H8 | 1.84 | 0.41 |
| 28:RF:122:LYS:HB3 | 28:RF:191:ARG:HA | 2.00 | 0.41 |
| 28:RF:67:GLN:O | 28:RF:67:GLN:HG3 | 2.20 | 0.41 |
| 29:RG:124:SER:OG | 29:RG:124:SER:O | 2.30 | 0.41 |
| 30:RH:58:GLU:OE1 | 30:RH:59:ARG:NH1 | 2.53 | 0.41 |
| 33:RO:50:GLY:H | 33:RO:53:LYS:HZ3 | 1.66 | 0.41 |
| 1:XA:1141:C:H2' | 1:XA:1142:G:C8 | 2.50 | 0.41 |
| 1:XA:1429:C:H2' | 1:XA:1430:C:C6 | 2.55 | 0.41 |
| 1:XA:339:C:H2' | 1:XA:340:U:H6 | 1.85 | 0.41 |
| 1:XA:1253:G:H4' | 10:XJ:46:ARG:HH22 | 1.85 | 0.41 |
| 24:YA:2365:G:O6 | 53:Y8:43:GLN:NE2 | 2.53 | 0.41 |
| 24:YA:108:U:H2' | 24:YA:109:G:H8 | 1.85 | 0.41 |
| 24:YA:1355:G:H2' | 24:YA:1356:G:H8 | 1.85 | 0.41 |
| 24:YA:1604:C:H2' | 24:YA:1605:C:H6 | 1.84 | 0.41 |
| 24:YA:1888:G:OP2 | 24:YA:1888:G:N2 | 2.53 | 0.41 |
| 24:YA:1268:A:OP1 | 24:YA:2006:C:OP1 | 2.37 | 0.41 |
| 24:YA:2566:A:H4' | 24:YA:2567:G:O5' | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 24:YA:2712:U:O2' | 24:YA:2712(A):A:OP1 | 2.38 | 0.41 |
| 27:YE:12:THR:OG1 | 27:YE:13:ARG:N | 2.53 | 0.41 |
| 34:YP:49:ARG:HG3 | 53:Y8:59:LYS:NZ | 2.35 | 0.41 |
| 39:YU:58:ARG:O | 39:YU:62:ILE:HG12 | 2.20 | 0.41 |
| 1:QA:10:A:H2' | 1:QA:11:G:C8 | 2.55 | 0.41 |
| 1:QA:627:G:H2' | 1:QA:628:G:H8 | 1.86 | 0.41 |
| 1:QA:812:C:H1' | 1:QA:813:U:OP2 | 2.20 | 0.41 |
| 1:QA:940:C:H2' | 1:QA:941:G:C8 | 2.55 | 0.41 |
| 1:QA:950:U:H2' | 1:QA:951:G:H8 | 1.85 | 0.41 |
| 7:QG:30:ILE:HG23 | 7:QG:39:ALA:HB1 | 2.02 | 0.41 |
| 24:RA:1289:C:H2' | 24:RA:1290:C:C6 | 2.54 | 0.41 |
| 24:RA:1794:U:H2' | 24:RA:1795:C:H6 | 1.84 | 0.41 |
| 24:RA:2036:C:H2' | 24:RA:2037:G:H8 | 1.85 | 0.41 |
| 24:RA:302:C:H2' | 24:RA:303:U:C6 | 2.55 | 0.41 |
| 24:RA:532:A:N1 | 24:RA:2035:G:N2 | 2.68 | 0.41 |
| 24:RA:903:C:H2' | 24:RA:904:C:H6 | 1.86 | 0.41 |
| 25:RB:109:G:H2' | 25:RB:110:G:H8 | 1.85 | 0.41 |
| 24:RA:2619:C:H5'' | 27:RE:152:LYS:HA | 2.01 | 0.41 |
| 30:RH:86:GLU:HB3 | 30:RH:165:ALA:H | 1.85 | 0.41 |
| 1:XA:1245:A:H2' | 1:XA:1246:C:C6 | 2.55 | 0.41 |
| 1:XA:1336:C:H1' | 1:XA:1337:G:C2 | 2.55 | 0.41 |
| 1:XA:408:A:OP2 | 4:XD:115:ARG:NH2 | 2.53 | 0.41 |
| 1:XA:663:A:H2' | 1:XA:664:G:C8 | 2.55 | 0.41 |
| 1:XA:762:C:H2' | 1:XA:763:G:C8 | 2.54 | 0.41 |
| 1:XA:913:A:H1' | 1:XA:914:A:OP2 | 2.19 | 0.41 |
| 17:XQ:81:ARG:NH1 | 17:XQ:83:ASP:OD2 | 2.53 | 0.41 |
| 18:XR:58:LEU:HD12 | 18:XR:62:GLU:HB3 | 2.01 | 0.41 |
| 24:YA:1065:U:H1' | 24:YA:1074:G:H22 | 1.85 | 0.41 |
| 24:YA:1535:U:N3 | 24:YA:1537:C:H1' | 2.35 | 0.41 |
| 24:YA:1728:G:H3' | 24:YA:1729:A:C5' | 2.50 | 0.41 |
| 24:YA:1748:G:H2' | 24:YA:1749:A:H8 | 1.86 | 0.41 |
| 24:YA:1791:A:H3' | 24:YA:1792:G:H8 | 1.86 | 0.41 |
| 24:YA:2342:C:O2' | 24:YA:2374:C:H5'' | 2.20 | 0.41 |
| 24:YA:2540:C:H2' | 24:YA:2541:A:O4' | 2.20 | 0.41 |
| 24:YA:2783:G:H2' | 24:YA:2784:C:C6 | 2.56 | 0.41 |
| 24:YA:279:C:H2' | 24:YA:280:C:H6 | 1.85 | 0.41 |
| 31:YI:78:THR:HG22 | 31:YI:141:LYS:HE2 | 2.01 | 0.41 |
| 1:QA:108:G:H5'' | 1:QA:109:A:H5'' | 2.03 | 0.41 |
| 1:QA:1152:A:H2' | 1:QA:1153:C:C6 | 2.55 | 0.41 |
| 1:QA:1330:U:OP2 | 1:QA:1330:U:H6 | 2.03 | 0.41 |
| 1:QA:137:C:H2' | 1:QA:138:G:C8 | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:33:A:H2' | 1:QA:34:C:C6 | 2.55 | 0.41 |
| 3:QC:124:ILE:HD12 | 3:QC:130:VAL:HG12 | 2.03 | 0.41 |
| 1:QA:619:U:N3 | 4:QD:134:ASP:OD1 | 2.35 | 0.41 |
| 12:QL:33:ARG:NH2 | 12:QL:61:THR:OG1 | 2.54 | 0.41 |
| 19:QS:32:LYS:HB3 | 19:QS:57:HIS:CE1 | 2.56 | 0.41 |
| 24:RA:1220:A:H5' | 24:RA:1221:C:OP2 | 2.20 | 0.41 |
| 24:RA:1550:C:H2' | 24:RA:1551:C:H6 | 1.84 | 0.41 |
| 24:RA:208:C:H2' | 24:RA:209:C:H6 | 1.85 | 0.41 |
| 24:RA:2133:G:N7 | 24:RA:2157:G:N1 | 2.68 | 0.41 |
| 24:RA:2210:G:H5' | 24:RA:2211:G:C5 | 2.55 | 0.41 |
| 24:RA:2773:C:OP1 | 27:RE:164:ARG:NE | 2.52 | 0.41 |
| 24:RA:2823:A:OP1 | 27:RE:113:PHE:HB2 | 2.21 | 0.41 |
| 24:RA:680:G:H2' | 24:RA:681:G:H8 | 1.85 | 0.41 |
| 25:RB:16:G:H2' | 25:RB:17:C:C6 | 2.55 | 0.41 |
| 28:RF:122:LYS:HB3 | 28:RF:191:ARG:HG3 | 2.02 | 0.41 |
| 29:RG:81:LYS:O | 29:RG:82:LEU:HB2 | 2.20 | 0.41 |
| 36:RR:22:ARG:HG2 | 36:RR:69:ASP:HB3 | 2.03 | 0.41 |
| 41:RW:111:HIS:HD2 | 41:RW:113:LYS:H | 1.68 | 0.41 |
| 41:RW:86:LEU:HD12 | 41:RW:96:ILE:HD11 | 2.02 | 0.41 |
| 1:XA:604:G:H2' | 1:XA:605:U:C6 | 2.55 | 0.41 |
| 1:XA:911:U:H2' | 1:XA:912:C:C6 | 2.55 | 0.41 |
| 12:XL:44:THR:HA | 12:XL:45:PRO:HD3 | 1.81 | 0.41 |
| 17:XQ:69:LYS:HA | 17:XQ:69:LYS:HD2 | 1.81 | 0.41 |
| 20:XT:92:LEU:HA | 20:XT:92:LEU:HD13 | 1.83 | 0.41 |
| 21:XU:12:LYS:HG2 | 21:XU:22:ARG:HB3 | 2.02 | 0.41 |
| 47:Y2:42:GLY:O | 47:Y2:44:LEU:N | 2.45 | 0.41 |
| 49:Y4:46:GLN:C | 49:Y4:48:ARG:H | 2.24 | 0.41 |
| 24:YA:142:G:H2' | 24:YA:143:C:C6 | 2.56 | 0.41 |
| 24:YA:1799:G:H5'' | 24:YA:1800:C:C5 | 2.55 | 0.41 |
| 24:YA:1812:A:H2' | 24:YA:1813:G:C8 | 2.54 | 0.41 |
| 24:YA:1791:A:N6 | 24:YA:1828:G:O2' | 2.46 | 0.41 |
| 24:YA:229:A:OP1 | 24:YA:229:A:H4' | 2.15 | 0.41 |
| 24:YA:2567:G:H2' | 24:YA:2568:C:C6 | 2.55 | 0.41 |
| 24:YA:2685:G:P | 38:YT:51:ARG:HH22 | 2.43 | 0.41 |
| 24:YA:2703:C:H2' | 24:YA:2704:C:H6 | 1.85 | 0.41 |
| 24:YA:440:G:H2' | 24:YA:441:U:C6 | 2.55 | 0.41 |
| 24:YA:463:G:N2 | 24:YA:466:A:OP2 | 2.51 | 0.41 |
| 24:YA:524:U:H2' | 24:YA:525:U:C6 | 2.55 | 0.41 |
| 26:YD:69:ARG:HD2 | 26:YD:105:ILE:HD13 | 2.02 | 0.41 |
| 36:YR:91:GLN:OE1 | 36:YR:91:GLN:N | 2.53 | 0.41 |
| 1:QA:407:G:H2' | 1:QA:408:A:C8 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:513:C:H2' | 1:QA:514:C:C6 | 2.55 | 0.41 |
| 1:QA:1100:C:OP2 | 2:QB:96:ARG:HD3 | 2.20 | 0.41 |
| 4:QD:68:TYR:HD2 | 4:QD:97:LEU:HD12 | 1.86 | 0.41 |
| 12:QL:93:LEU:HA | 12:QL:93:LEU:HD13 | 1.85 | 0.41 |
| 23:QX:15:A:H4' | 23:QX:16:A:OP2 | 2.19 | 0.41 |
| 45:R0:68:GLU:OE2 | 45:R0:82:ARG:NH1 | 2.53 | 0.41 |
| 53:R8:50:LEU:HD12 | 53:R8:51:ALA:H | 1.84 | 0.41 |
| 24:RA:1400:G:H2' | 24:RA:1401:G:H8 | 1.85 | 0.41 |
| 24:RA:1551:C:H2' | 24:RA:1552:G:O4' | 2.20 | 0.41 |
| 24:RA:1656:C:H2' | 24:RA:1657:C:H6 | 1.85 | 0.41 |
| 24:RA:2060:A:H4' | 24:RA:2061:G:OP2 | 2.21 | 0.41 |
| 24:RA:2649:U:H2' | 24:RA:2650:U:C6 | 2.56 | 0.41 |
| 24:RA:321:G:OP2 | 28:RF:135:LYS:HD3 | 2.21 | 0.41 |
| 29:RG:15:VAL:HG11 | 29:RG:176:LEU:HD22 | 2.02 | 0.41 |
| 1:XA:325:A:OP2 | 20:XT:70:SER:OG | 2.18 | 0.41 |
| 1:XA:370:C:H2' | 1:XA:371:G:C8 | 2.56 | 0.41 |
| 1:XA:437:U:H2' | 1:XA:438:G:O4' | 2.21 | 0.41 |
| 1:XA:481:G:O2' | 1:XA:482:A:C8 | 2.72 | 0.41 |
| 1:XA:485:G:HO2' | 1:XA:486:U:P | 2.44 | 0.41 |
| 14:XN:32:SER:HB3 | 14:XN:41:ARG:HD2 | 2.02 | 0.41 |
| 14:XN:34:TYR:HD1 | 14:XN:44:LEU:HD21 | 1.86 | 0.41 |
| 24:YA:1539:G:H2' | 24:YA:1540:G:H8 | 1.84 | 0.41 |
| 24:YA:1588:C:H2' | 24:YA:1589:C:C6 | 2.55 | 0.41 |
| 24:YA:1821:A:H2' | 24:YA:1822:G:C8 | 2.55 | 0.41 |
| 24:YA:2065:C:H2' | 24:YA:2066:C:C6 | 2.55 | 0.41 |
| 24:YA:2448:A:OP2 | 24:YA:2499:C:P | 2.79 | 0.41 |
| 24:YA:2514:U:H2' | 24:YA:2515:C:H6 | 1.85 | 0.41 |
| 24:YA:2611:U:P | 24:YA:2611:U:H3' | 2.61 | 0.41 |
| 24:YA:2773:C:H2' | 24:YA:2774:C:H6 | 1.85 | 0.41 |
| 24:YA:286:C:H2' | 24:YA:287:C:H6 | 1.86 | 0.41 |
| 24:YA:546:C:H5'' | 24:YA:547:A:N7 | 2.36 | 0.41 |
| 24:YA:465:G:H21 | 24:YA:684:G:H1' | 1.84 | 0.41 |
| 24:YA:774:A:H2 | 24:YA:787:U:HO2' | 1.65 | 0.41 |
| 26:YD:77:ALA:HB3 | 26:YD:117:VAL:HG13 | 2.02 | 0.41 |
| 29:YG:27:ASN:OD1 | 29:YG:28:VAL:N | 2.53 | 0.41 |
| 37:YS:66:ALA:HA | 37:YS:69:VAL:HG12 | 2.02 | 0.41 |
| 40:YV:14:VAL:HB | 40:YV:96:ILE:HG13 | 2.01 | 0.41 |
| 4:QD:116:GLN:O | 4:QD:120:LEU:HG | 2.21 | 0.41 |
| 4:QD:191:ARG:HD2 | 4:QD:192:GLU:N | 2.35 | 0.41 |
| 16:QP:69:THR:O | 16:QP:73:LEU:HD23 | 2.21 | 0.41 |
| 24:RA:1065:U:H5'' | 24:RA:1066:U:C6 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:RA:1561:G:H2' | 24:RA:1562:A:C8 | 2.55 | 0.41 |
| 24:RA:407:G:H2' | 24:RA:408:G:C8 | 2.55 | 0.41 |
| 24:RA:690:G:H2' | 24:RA:691:C:C6 | 2.56 | 0.41 |
| 27:RE:144:ARG:HB3 | 27:RE:145:LYS:H | 1.77 | 0.41 |
| 29:RG:176:LEU:HD13 | 29:RG:176:LEU:HA | 1.89 | 0.41 |
| 31:RI:93:THR:OG1 | 31:RI:94:ALA:N | 2.53 | 0.41 |
| 41:RW:36:LEU:HD13 | 41:RW:47:VAL:HG23 | 2.02 | 0.41 |
| 1:XA:1454:G:H2' | 1:XA:1455:G:H8 | 1.86 | 0.41 |
| 1:XA:7:G:H5' | 1:XA:298:A:O4' | 2.20 | 0.41 |
| 10:XJ:48:THR:HG23 | 10:XJ:62:HIS:HB3 | 2.03 | 0.41 |
| 10:XJ:39:PRO:HA | 10:XJ:70:ARG:NE | 2.36 | 0.41 |
| 10:XJ:79:ARG:HA | 10:XJ:82:ILE:HB | 2.02 | 0.41 |
| 15:XO:43:LEU:HD11 | 24:YA:715:G:H22 | 1.85 | 0.41 |
| 46:Y1:53:VAL:C | 46:Y1:55:GLY:H | 2.23 | 0.41 |
| 24:YA:1291:C:H2' | 24:YA:1292:U:C6 | 2.55 | 0.41 |
| 24:YA:1825:A:H2' | 24:YA:1826:G:C8 | 2.56 | 0.41 |
| 24:YA:2514:U:H3 | 24:YA:2570:G:H1 | 1.66 | 0.41 |
| 24:YA:514:A:H2' | 24:YA:515:A:C8 | 2.55 | 0.41 |
| 24:YA:907:U:O2' | 35:YQ:101:ARG:NH2 | 2.51 | 0.41 |
| 30:YH:119:GLU:O | 30:YH:140:LYS:NZ | 2.39 | 0.41 |
| 34:YP:6:LEU:HD13 | 34:YP:6:LEU:HA | 1.91 | 0.41 |
| 24:YA:2318:G:N2 | 37:YS:3:ARG:HE | 2.18 | 0.41 |
| 1:QA:1314:C:H2' | 1:QA:1315:U:C6 | 2.56 | 0.41 |
| 1:QA:1336:C:O2' | 1:QA:1337:G:O5' | 2.37 | 0.41 |
| 1:QA:1351:U:H3 | 1:QA:1371:G:H1 | 1.68 | 0.41 |
| 1:QA:404:U:H5'' | 4:QD:122:ARG:HH11 | 1.86 | 0.41 |
| 1:QA:584:G:H2' | 1:QA:585:G:H8 | 1.85 | 0.41 |
| 1:QA:587:G:OP1 | 8:QH:92:ARG:NH2 | 2.48 | 0.41 |
| 3:QC:150:LYS:HB2 | 3:QC:201:TYR:HB2 | 2.03 | 0.41 |
| 7:QG:115:ARG:HB3 | 7:QG:118:VAL:HG22 | 2.02 | 0.41 |
| 7:QG:62:PHE:HA | 7:QG:124:LEU:HD12 | 2.03 | 0.41 |
| 13:QM:23:TYR:HD2 | 13:QM:67:GLU:HA | 1.86 | 0.41 |
| 20:QT:54:LYS:NZ | 20:QT:100:ILE:HG21 | 2.36 | 0.41 |
| 24:RA:2347:C:HO2' | 51:R6:21:TYR:HH | 1.59 | 0.41 |
| 24:RA:1562:A:H2' | 24:RA:1563:G:C8 | 2.56 | 0.41 |
| 24:RA:1600:C:OP1 | 42:RX:58:HIS:NE2 | 2.38 | 0.41 |
| 24:RA:1653:G:H1' | 24:RA:1654:A:OP2 | 2.21 | 0.41 |
| 24:RA:807:U:O2' | 24:RA:2060:A:N1 | 2.44 | 0.41 |
| 24:RA:2648:C:H2' | 24:RA:2649:U:H6 | 1.86 | 0.41 |
| 24:RA:309:G:H8 | 24:RA:309:G:P | 2.44 | 0.41 |
| 24:RA:407:G:H2' | 24:RA:408:G:H8 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:RA:415:A:H2' | 24:RA:416:C:H6 | 1.85 | 0.41 |
| 24:RA:448:U:C4 | 24:RA:583:G:H1' | 2.56 | 0.41 |
| 24:RA:623:G:H2' | 24:RA:624:C:C6 | 2.55 | 0.41 |
| 30:RH:30:LYS:HD2 | 30:RH:30:LYS:HA | 1.80 | 0.41 |
| 30:RH:4:ILE:HB | 30:RH:6:ARG:NH1 | 2.35 | 0.41 |
| 1:XA:1408:A:C6 | 1:XA:1494:G:N1 | 2.89 | 0.41 |
| 1:XA:93:U:H2' | 1:XA:95:G:O4' | 2.20 | 0.41 |
| 8:XH:69:ARG:NH2 | 8:XH:75:ARG:O | 2.54 | 0.41 |
| 10:XJ:34:VAL:HG12 | 10:XJ:74:ILE:HG12 | 2.02 | 0.41 |
| 12:XL:85:ILE:HA | 12:XL:85:ILE:HD12 | 1.98 | 0.41 |
| 10:XJ:62:HIS:ND1 | 14:XN:59:ALA:HB3 | 2.34 | 0.41 |
| 1:XA:1229:A:O2' | 22:XV:31:C:OP1 | 2.37 | 0.41 |
| 25:YB:83:G:H4' | 48:Y3:52:HIS:CG | 2.55 | 0.41 |
| 24:YA:147:U:H2' | 24:YA:148:C:C6 | 2.56 | 0.41 |
| 24:YA:2105:C:H2' | 24:YA:2106:G:C8 | 2.55 | 0.41 |
| 24:YA:740:U:H2' | 24:YA:741:G:H8 | 1.86 | 0.41 |
| 24:YA:742:G:H2' | 24:YA:743:G:C8 | 2.55 | 0.41 |
| 24:YA:78:A:H2' | 24:YA:79:G:H8 | 1.85 | 0.41 |
| 24:YA:962:G:H2' | 24:YA:963:U:C6 | 2.56 | 0.41 |
| 28:YF:24:LEU:HD23 | 28:YF:115:ALA:HA | 2.02 | 0.41 |
| 24:YA:1131:G:H4' | 32:YN:82:LEU:HD12 | 2.01 | 0.41 |
| 34:YP:94:GLU:O | 34:YP:96:THR:HG23 | 2.21 | 0.41 |
| 35:YQ:116:GLU:OE2 | 35:YQ:119:ARG:NH2 | 2.38 | 0.41 |
| 24:YA:1754:C:H5' | 38:YT:101:PHE:CZ | 2.56 | 0.41 |
| 24:YA:1614:A:C6 | 41:YW:91:GLY:HA2 | 2.56 | 0.41 |
| 44:YZ:118:GLN:HG2 | 44:YZ:120:ILE:HD13 | 2.02 | 0.41 |
| 1:QA:1059:C:H2' | 1:QA:1060:C:C6 | 2.55 | 0.41 |
| 1:QA:1129:C:H4' | 1:QA:1130:A:H8 | 1.85 | 0.41 |
| 1:QA:1191:A:H5'' | 3:QC:4:LYS:HE3 | 2.03 | 0.41 |
| 1:QA:1384:C:H2' | 1:QA:1385:G:H8 | 1.85 | 0.41 |
| 1:QA:272:C:H2' | 1:QA:273:A:C8 | 2.50 | 0.41 |
| 1:QA:309:G:H2' | 1:QA:310:G:H8 | 1.86 | 0.41 |
| 1:QA:343:U:O2 | 1:QA:347:G:C6 | 2.74 | 0.41 |
| 1:QA:674:G:H2' | 1:QA:675:A:C8 | 2.43 | 0.41 |
| 6:QF:46:ARG:HH21 | 18:QR:37:VAL:HG11 | 1.85 | 0.41 |
| 8:QH:38:ILE:HG21 | 8:QH:111:ILE:HD13 | 2.03 | 0.41 |
| 9:QI:3:GLN:HG3 | 9:QI:20:ARG:HD3 | 2.02 | 0.41 |
| 9:QI:4:TYR:CE1 | 9:QI:87:GLN:HG3 | 2.55 | 0.41 |
| 13:QM:17:VAL:HA | 13:QM:20:THR:CG2 | 2.51 | 0.41 |
| 18:QR:70:ILE:O | 18:QR:74:ARG:HB2 | 2.20 | 0.41 |
| 24:RA:1278:A:H2' | 24:RA:1279:G:C8 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:RA:1952:A:N3 | 24:RA:2560:C:O2' | 2.40 | 0.41 |
| 24:RA:2037:G:H2' | 24:RA:2038:G:H8 | 1.85 | 0.41 |
| 24:RA:2065:C:H2' | 24:RA:2066:C:H6 | 1.86 | 0.41 |
| 24:RA:2314:C:H2' | 24:RA:2315:G:C8 | 2.56 | 0.41 |
| 24:RA:2728:U:H2' | 24:RA:2729:G:H8 | 1.85 | 0.41 |
| 24:RA:2863:C:H2' | 24:RA:2864:G:H8 | 1.86 | 0.41 |
| 24:RA:2892:A:H2' | 24:RA:2893:G:O4' | 2.20 | 0.41 |
| 24:RA:2891:G:H5' | 24:RA:2892:A:OP1 | 2.21 | 0.41 |
| 24:RA:935:C:H2' | 24:RA:936:C:C6 | 2.56 | 0.41 |
| 24:RA:1656:C:P | 27:RE:136:ARG:HE | 2.43 | 0.41 |
| 27:RE:34:VAL:HG21 | 27:RE:77:ILE:HD11 | 2.01 | 0.41 |
| 28:RF:198:ALA:N | 28:RF:200:GLU:OE2 | 2.53 | 0.41 |
| 29:RG:133:LEU:HA | 29:RG:133:LEU:HD23 | 1.93 | 0.41 |
| 34:RP:138:LEU:HD21 | 34:RP:144:GLU:HB3 | 2.03 | 0.41 |
| 1:XA:1095:U:P | 1:XA:1108:G:H1 | 2.43 | 0.41 |
| 1:XA:1409:C:H2' | 1:XA:1410:G:C8 | 2.54 | 0.41 |
| 1:XA:195:A:H2' | 1:XA:196:A:C4 | 2.55 | 0.41 |
| 2:XB:161:ALA:HA | 2:XB:183:PRO:O | 2.21 | 0.41 |
| 8:XH:49:GLU:HG2 | 8:XH:62:TYR:HE2 | 1.86 | 0.41 |
| 9:XI:10:ARG:NH1 | 9:XI:75:ASP:OD1 | 2.54 | 0.41 |
| 1:XA:1280:A:P | 10:XJ:40:LEU:HD21 | 2.61 | 0.41 |
| 11:XK:120:ARG:HA | 11:XK:121:PRO:HD3 | 1.88 | 0.41 |
| 14:XN:47:LEU:HD13 | 14:XN:50:LYS:HD3 | 2.02 | 0.41 |
| 1:XA:247:G:OP2 | 17:XQ:100:LYS:HG3 | 2.21 | 0.41 |
| 20:XT:61:SER:O | 20:XT:65:LYS:HG3 | 2.21 | 0.41 |
| 46:Y1:5:CYS:HG | 46:Y1:8:SER:HG | 1.67 | 0.41 |
| 24:YA:108:U:H2' | 24:YA:109:G:C8 | 2.55 | 0.41 |
| 24:YA:1111:A:OP1 | 30:YH:3:ARG:NH2 | 2.53 | 0.41 |
| 24:YA:1252:G:H1 | 39:YU:37:GLU:HG3 | 1.85 | 0.41 |
| 24:YA:1293:C:H2' | 24:YA:1294:U:C6 | 2.56 | 0.41 |
| 24:YA:1423:G:H2' | 24:YA:1424:G:H8 | 1.85 | 0.41 |
| 24:YA:2229:C:H2' | 24:YA:2230:G:H8 | 1.85 | 0.41 |
| 24:YA:278:A:H2' | 24:YA:279:C:C6 | 2.56 | 0.41 |
| 24:YA:84:A:OP2 | 43:YY:8:LYS:NZ | 2.48 | 0.41 |
| 1:QA:954:G:H21 | 1:QA:1227:A:H62 | 1.67 | 0.41 |
| 1:QA:279:A:OP1 | 1:QA:280:C:O2' | 2.23 | 0.41 |
| 1:QA:501:C:OP1 | 12:QL:117:ARG:NH2 | 2.54 | 0.41 |
| 2:QB:115:LEU:HD13 | 2:QB:145:LEU:HG | 2.02 | 0.41 |
| 4:QD:98:GLU:HA | 4:QD:103:ASN:ND2 | 2.35 | 0.41 |
| 13:QM:51:ALA:HA | 13:QM:54:VAL:HG12 | 2.03 | 0.41 |
| 20:QT:54:LYS:HZ1 | 20:QT:100:ILE:HG21 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:RA:2020:A:H5' | 50:R5:12:SER:HB3 | 2.02 | 0.41 |
| 51:R6:23:THR:OG1 | 51:R6:24:GLU:N | 2.54 | 0.41 |
| 24:RA:99:U:H4' | 24:RA:101:G:O5' | 2.19 | 0.41 |
| 24:RA:1568:G:OP2 | 26:RD:63:ARG:NH2 | 2.48 | 0.41 |
| 24:RA:2618:G:H21 | 27:RE:150:VAL:HG21 | 1.85 | 0.41 |
| 24:RA:2676:C:H2' | 24:RA:2677:G:C8 | 2.56 | 0.41 |
| 24:RA:270(Y):G:H2' | 24:RA:270(Z):U:C6 | 2.56 | 0.41 |
| 24:RA:2747:G:H21 | 24:RA:2757:A:N6 | 2.13 | 0.41 |
| 24:RA:52:A:H2' | 24:RA:53:A:C8 | 2.56 | 0.41 |
| 25:RB:28:C:H2' | 25:RB:29:A:H8 | 1.86 | 0.41 |
| 27:RE:92:THR:OG1 | 27:RE:93:VAL:N | 2.53 | 0.41 |
| 34:RP:101:VAL:HB | 34:RP:106:LEU:HB2 | 2.03 | 0.41 |
| 39:RU:91:ASP:C | 39:RU:93:LYS:H | 2.24 | 0.41 |
| 43:RY:17:SER:OG | 43:RY:71:LYS:NZ | 2.41 | 0.41 |
| 1:XA:1029:G:O2' | 1:XA:1032(A):G:N2 | 2.38 | 0.41 |
| 1:XA:1515:C:H2' | 1:XA:1516:G:C8 | 2.56 | 0.41 |
| 1:XA:536:C:H2' | 1:XA:537:G:H8 | 1.85 | 0.41 |
| 1:XA:986:A:H4' | 19:XS:55:LYS:NZ | 2.36 | 0.41 |
| 2:XB:27:LYS:HA | 2:XB:27:LYS:HD2 | 1.83 | 0.41 |
| 4:XD:126:ILE:HG22 | 4:XD:146:ILE:HD11 | 2.03 | 0.41 |
| 4:XD:108:LEU:HD23 | 4:XD:174:LEU:HD13 | 2.02 | 0.41 |
| 12:XL:62:SER:O | 12:XL:62:SER:OG | 2.34 | 0.41 |
| 17:XQ:50:LYS:HE3 | 17:XQ:51:TYR:CZ | 2.55 | 0.41 |
| 24:YA:1079:C:H2' | 24:YA:1080:C:C6 | 2.55 | 0.41 |
| 24:YA:1167:U:H2' | 24:YA:1168:G:H8 | 1.86 | 0.41 |
| 24:YA:1709:U:H2' | 24:YA:1710:C:C6 | 2.56 | 0.41 |
| 24:YA:1790:C:H2' | 24:YA:1791:A:C5 | 2.56 | 0.41 |
| 24:YA:1871:A:OP2 | 24:YA:1871:A:H8 | 2.04 | 0.41 |
| 24:YA:2695:C:H2' | 24:YA:2696:U:C6 | 2.56 | 0.41 |
| 24:YA:2712:U:H6 | 24:YA:2712:U:H2' | 1.65 | 0.41 |
| 24:YA:2788:C:H4' | 24:YA:2809:A:O2' | 2.21 | 0.41 |
| 24:YA:447:A:C4' | 24:YA:449:A:N7 | 2.83 | 0.41 |
| 24:YA:669:G:N3 | 24:YA:669:G:H2' | 2.36 | 0.41 |
| 24:YA:781:A:OP1 | 26:YD:218:ARG:NH2 | 2.54 | 0.41 |
| 24:YA:936:C:H2' | 24:YA:937:U:C6 | 2.56 | 0.41 |
| 24:YA:729:G:OP2 | 26:YD:13:ARG:HD3 | 2.21 | 0.41 |
| 33:YO:88:ASN:HD21 | 33:YO:92:GLU:HB2 | 1.86 | 0.41 |
| 1:QA:1277:C:O2' | 1:QA:1279:A:H8 | 2.03 | 0.41 |
| 1:QA:17:U:H2' | 1:QA:18:C:H6 | 1.86 | 0.41 |
| 1:QA:404:U:H2' | 1:QA:405:U:H6 | 1.86 | 0.41 |
| 1:QA:924:C:H2' | 1:QA:925:G:H8 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:QE:94:ALA:HB2 | 5:QE:119:LEU:HG | 2.03 | 0.41 |
| 7:QG:92:SER:O | 7:QG:96:GLN:HG3 | 2.21 | 0.41 |
| 16:QP:53:VAL:HG13 | 16:QP:79:VAL:HG22 | 2.02 | 0.41 |
| 24:RA:1680:U:H2' | 24:RA:1681:G:O4' | 2.20 | 0.41 |
| 24:RA:1889:A:H2' | 24:RA:1890:A:C8 | 2.56 | 0.41 |
| 24:RA:2342:C:O2' | 24:RA:2374:C:H5'' | 2.20 | 0.41 |
| 24:RA:2345:G:O2' | 24:RA:2381:C:O2 | 2.32 | 0.41 |
| 24:RA:2600:A:H2' | 24:RA:2601:C:C6 | 2.56 | 0.41 |
| 24:RA:2841:C:H2' | 24:RA:2842:G:C8 | 2.56 | 0.41 |
| 24:RA:297:C:OP1 | 43:RY:87:LYS:HE3 | 2.20 | 0.41 |
| 24:RA:811:U:H2' | 34:RP:21:ARG:O | 2.21 | 0.41 |
| 26:RD:83:GLU:HB2 | 26:RD:92:ILE:HD11 | 2.03 | 0.41 |
| 28:RF:116:ASP:OD1 | 28:RF:119:ARG:NH2 | 2.54 | 0.41 |
| 29:RG:60:LEU:HD22 | 29:RG:68:PRO:HB3 | 2.03 | 0.41 |
| 30:RH:62:LYS:HE2 | 30:RH:62:LYS:HB3 | 1.91 | 0.41 |
| 43:RY:63:LYS:HD3 | 43:RY:64:GLU:N | 2.36 | 0.41 |
| 1:XA:1187:G:H5' | 1:XA:1188:A:OP2 | 2.20 | 0.41 |
| 1:XA:1388:C:H2' | 1:XA:1389:C:C6 | 2.56 | 0.41 |
| 1:XA:582:U:H2' | 1:XA:583:A:H8 | 1.85 | 0.41 |
| 1:XA:646:U:H2' | 1:XA:647:C:C6 | 2.56 | 0.41 |
| 1:XA:923:A:H2' | 1:XA:924:C:C6 | 2.56 | 0.41 |
| 2:XB:114:ARG:HA | 2:XB:114:ARG:HD2 | 1.83 | 0.41 |
| 2:XB:47:THR:O | 2:XB:51:LEU:HG | 2.19 | 0.41 |
| 17:XQ:19:VAL:HG23 | 17:XQ:44:ALA:HB3 | 2.02 | 0.41 |
| 49:Y4:49:PHE:HD2 | 49:Y4:49:PHE:H | 1.68 | 0.41 |
| 24:YA:110:G:H2' | 24:YA:111:A:H8 | 1.86 | 0.41 |
| 24:YA:137(A):G:H2' | 24:YA:139:G:N7 | 2.36 | 0.41 |
| 24:YA:1710:C:H2' | 24:YA:1711:C:H6 | 1.86 | 0.41 |
| 24:YA:1820:U:C2 | 26:YD:202:LYS:HB2 | 2.56 | 0.41 |
| 24:YA:2291:U:O2' | 24:YA:2374:C:O2 | 2.39 | 0.41 |
| 24:YA:265:A:N6 | 24:YA:427:U:HO2' | 2.19 | 0.41 |
| 24:YA:642:G:H21 | 24:YA:646:A:H2 | 1.67 | 0.41 |
| 29:YG:43:LEU:HA | 29:YG:43:LEU:HD13 | 1.91 | 0.41 |
| 30:YH:86:GLU:HB3 | 30:YH:165:ALA:H | 1.86 | 0.41 |
| 44:YZ:24:LEU:HD21 | 44:YZ:86:VAL:HG13 | 2.03 | 0.41 |
| 1:QA:1150:U:O4 | 1:QA:1151:A:N6 | 2.54 | 0.41 |
| 1:QA:1347:G:O6 | 9:QI:10:ARG:NH2 | 2.40 | 0.41 |
| 1:QA:1404:C:H2' | 1:QA:1405:G:C8 | 2.55 | 0.41 |
| 1:QA:163:C:H2' | 1:QA:164:U:H6 | 1.86 | 0.41 |
| 1:QA:17:U:H2' | 1:QA:18:C:C6 | 2.56 | 0.41 |
| 1:QA:192:U:H2' | 1:QA:193:C:C6 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:QD:119:GLN:HA | 4:QD:122:ARG:HG2 | 2.02 | 0.41 |
| 5:QE:91:LEU:HD13 | 5:QE:120:THR:HG22 | 2.02 | 0.41 |
| 1:QA:1342:C:H1' | 9:QI:124:GLN:NE2 | 2.36 | 0.41 |
| 10:QJ:50:ILE:HA | 10:QJ:60:ARG:HG2 | 2.02 | 0.41 |
| 13:QM:66:LEU:HD13 | 13:QM:66:LEU:HA | 1.72 | 0.41 |
| 17:QQ:45:HIS:CD2 | 17:QQ:47:PRO:HG3 | 2.56 | 0.41 |
| 45:R0:70:GLN:O | 45:R0:78:TYR:N | 2.51 | 0.41 |
| 46:R1:82:LEU:HA | 46:R1:82:LEU:HD23 | 1.97 | 0.41 |
| 24:RA:1106:G:H2' | 24:RA:1107:G:C8 | 2.56 | 0.41 |
| 24:RA:1184:G:OP1 | 48:R3:29:ARG:NH1 | 2.54 | 0.41 |
| 24:RA:1657:C:H2' | 24:RA:1658:C:C6 | 2.55 | 0.41 |
| 24:RA:280:C:H2' | 24:RA:281:G:O4' | 2.21 | 0.41 |
| 24:RA:93:C:H2' | 24:RA:94:G:O4' | 2.21 | 0.41 |
| 30:RH:107:VAL:HG21 | 30:RH:151:ILE:HG21 | 2.02 | 0.41 |
| 33:RO:22:ILE:HG13 | 33:RO:41:ALA:HA | 2.02 | 0.41 |
| 27:RE:20:ALA:N | 33:RO:72:PRO:O | 2.48 | 0.41 |
| 35:RQ:122:GLY:HA2 | 35:RQ:129:THR:HG21 | 2.03 | 0.41 |
| 43:RY:53:PRO:C | 43:RY:55:TYR:H | 2.24 | 0.41 |
| 44:RZ:131:ARG:H | 44:RZ:131:ARG:HD2 | 1.85 | 0.41 |
| 44:RZ:35:ARG:HA | 44:RZ:35:ARG:HD3 | 1.86 | 0.41 |
| 1:XA:1061:G:OP1 | 10:XJ:59:SER:OG | 2.37 | 0.41 |
| 1:XA:1145:C:H4' | 1:XA:1146:A:H8 | 1.86 | 0.41 |
| 1:XA:1427:U:H2' | 1:XA:1428:A:H8 | 1.86 | 0.41 |
| 1:XA:363:A:H2' | 1:XA:364:A:C8 | 2.56 | 0.41 |
| 1:XA:406:G:H2' | 1:XA:407:G:H8 | 1.84 | 0.41 |
| 1:XA:738:C:H2' | 1:XA:739:C:C6 | 2.56 | 0.41 |
| 1:XA:958:A:C6 | 19:XS:55:LYS:HB2 | 2.55 | 0.41 |
| 3:XC:184:TYR:HD2 | 3:XC:201:TYR:HE2 | 1.69 | 0.41 |
| 46:Y1:49:VAL:HG11 | 46:Y1:70:VAL:HG11 | 2.02 | 0.41 |
| 51:Y6:44:ARG:O | 51:Y6:45:LYS:HD3 | 2.21 | 0.41 |
| 24:YA:1566:A:OP2 | 26:YD:211:ARG:NH2 | 2.47 | 0.41 |
| 24:YA:1728:G:H3' | 24:YA:1729:A:H5'' | 2.02 | 0.41 |
| 24:YA:2734:A:H5' | 24:YA:2735:G:OP2 | 2.20 | 0.41 |
| 24:YA:2823:A:OP1 | 27:YE:113:PHE:HB2 | 2.21 | 0.41 |
| 25:YB:44:G:H5'' | 25:YB:45:A:OP1 | 2.21 | 0.41 |
| 29:YG:107:LEU:HD21 | 29:YG:178:PHE:CE1 | 2.56 | 0.41 |
| 30:YH:19:VAL:HA | 30:YH:24:VAL:HG12 | 2.04 | 0.41 |
| 32:YN:30:ILE:HG22 | 32:YN:34:LEU:HD23 | 2.02 | 0.41 |
| 42:YX:35:THR:O | 42:YX:39:ILE:HG13 | 2.21 | 0.41 |
| 1:QA:1059:C:H2' | 1:QA:1060:C:H6 | 1.86 | 0.40 |
| 1:QA:1414:U:H2' | 1:QA:1415:G:C8 | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:QA:167:G:H2' | 1:QA:168:G:H8 | 1.86 | 0.40 |
| 1:QA:321:A:H2' | 1:QA:322:C:C6 | 2.56 | 0.40 |
| 2:QB:16:HIS:HD2 | 2:QB:210:SER:HA | 1.85 | 0.40 |
| 6:QF:94:GLN:OE1 | 18:QR:32:ARG:NH1 | 2.49 | 0.40 |
| 12:QL:104:VAL:HG12 | 12:QL:107:ALA:HB3 | 2.04 | 0.40 |
| 12:QL:27:LEU:HA | 12:QL:27:LEU:HD12 | 1.82 | 0.40 |
| 1:QA:1314:C:N4 | 19:QS:2:PRO:O | 2.54 | 0.40 |
| 20:QT:81:LYS:O | 20:QT:85:MET:HG2 | 2.20 | 0.40 |
| 49:R4:16:CYS:SG | 49:R4:17:GLY:N | 2.95 | 0.40 |
| 24:RA:142:G:H2' | 24:RA:143:C:H6 | 1.86 | 0.40 |
| 24:RA:270(W):G:H2' | 24:RA:270(X):G:C8 | 2.56 | 0.40 |
| 24:RA:455:C:O2' | 24:RA:456:C:H5' | 2.21 | 0.40 |
| 24:RA:519:U:H2' | 24:RA:520:G:H8 | 1.86 | 0.40 |
| 25:RB:42:C:O2 | 29:RG:93:THR:N | 2.45 | 0.40 |
| 25:RB:86:G:H2' | 25:RB:87:G:H8 | 1.86 | 0.40 |
| 30:RH:55:PRO:HG2 | 30:RH:61:HIS:CE1 | 2.56 | 0.40 |
| 35:RQ:62:GLY:HA3 | 35:RQ:107:ALA:O | 2.21 | 0.40 |
| 37:RS:25:ARG:HB3 | 37:RS:40:ILE:HG23 | 2.02 | 0.40 |
| 40:RV:24:LYS:HA | 40:RV:92:THR:HG23 | 2.02 | 0.40 |
| 42:RX:21:PHE:HE1 | 42:RX:92:LEU:HB3 | 1.86 | 0.40 |
| 1:XA:105:G:H2' | 1:XA:106:C:C6 | 2.56 | 0.40 |
| 1:XA:1310:G:HO2' | 1:XA:1311:G:P | 2.44 | 0.40 |
| 1:XA:438:G:H4' | 4:XD:123:HIS:CD2 | 2.56 | 0.40 |
| 5:XE:147:ASP:O | 5:XE:151:LEU:HD23 | 2.21 | 0.40 |
| 14:XN:43:CYS:C | 14:XN:45:ARG:H | 2.25 | 0.40 |
| 24:YA:1411:C:H3' | 24:YA:1412:A:H8 | 1.86 | 0.40 |
| 24:YA:1444:G:H2' | 24:YA:1445:C:C5 | 2.56 | 0.40 |
| 24:YA:2323:G:H1 | 24:YA:2332:U:H3 | 1.68 | 0.40 |
| 24:YA:2339:G:H2' | 24:YA:2340:G:C8 | 2.57 | 0.40 |
| 24:YA:2647:U:H2' | 24:YA:2648:C:C6 | 2.56 | 0.40 |
| 24:YA:2863:C:H2' | 24:YA:2864:G:C8 | 2.56 | 0.40 |
| 24:YA:286:C:H2' | 24:YA:287:C:C6 | 2.56 | 0.40 |
| 24:YA:327:G:H2' | 24:YA:328:U:C6 | 2.55 | 0.40 |
| 27:YE:185:LYS:HA | 27:YE:185:LYS:HD2 | 1.84 | 0.40 |
| 28:YF:152:GLU:OE2 | 28:YF:152:GLU:N | 2.54 | 0.40 |
| 32:YN:114:ARG:O | 32:YN:115:ARG:HB3 | 2.21 | 0.40 |
| 39:YU:61:TRP:HB3 | 39:YU:93:LYS:O | 2.21 | 0.40 |
| 40:YV:5:VAL:HB | 40:YV:35:LEU:HD11 | 2.03 | 0.40 |
| 41:YW:33:ARG:NH2 | 41:YW:52:GLU:OE1 | 2.50 | 0.40 |
| 1:QA:1314:C:H2' | 1:QA:1315:U:H6 | 1.86 | 0.40 |
| 1:QA:381:C:H2' | 1:QA:382:A:O4' | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:QA:819:A:N7 | 1:QA:1529:G:N1 | 2.69 | 0.40 |
| 1:QA:939:G:H2' | 1:QA:940:C:C6 | 2.55 | 0.40 |
| 2:QB:114:ARG:O | 2:QB:118:LEU:HG | 2.22 | 0.40 |
| 4:QD:156:GLU:N | 4:QD:156:GLU:OE1 | 2.45 | 0.40 |
| 16:QP:19:ILE:O | 16:QP:36:ILE:HG22 | 2.21 | 0.40 |
| 34:RP:62:LEU:HD12 | 53:R8:30:ARG:HE | 1.86 | 0.40 |
| 53:R8:50:LEU:C | 53:R8:52:LYS:H | 2.25 | 0.40 |
| 24:RA:1847:A:H5' | 24:RA:1848:A:OP2 | 2.21 | 0.40 |
| 24:RA:1921:G:H2' | 24:RA:1922:G:H8 | 1.86 | 0.40 |
| 24:RA:270(U):C:H2' | 24:RA:270(V):G:C8 | 2.56 | 0.40 |
| 24:RA:587:C:H4' | 24:RA:588:U:O5' | 2.20 | 0.40 |
| 24:RA:634:C:H2' | 24:RA:635:C:H6 | 1.86 | 0.40 |
| 26:RD:182:LEU:HB2 | 26:RD:271:ILE:HB | 2.03 | 0.40 |
| 32:RN:112:LEU:HD12 | 32:RN:112:LEU:HA | 1.93 | 0.40 |
| 34:RP:7:ARG:HA | 34:RP:8:PRO:HD2 | 1.94 | 0.40 |
| 41:RW:60:ASN:O | 41:RW:61:ASN:ND2 | 2.53 | 0.40 |
| 1:XA:1036:G:H5' | 1:XA:1037:C:OP2 | 2.20 | 0.40 |
| 1:XA:1412:C:H2' | 1:XA:1413:A:H8 | 1.86 | 0.40 |
| 1:XA:19:C:H2' | 1:XA:20:U:H6 | 1.86 | 0.40 |
| 1:XA:777:A:H2' | 1:XA:778:G:C8 | 2.56 | 0.40 |
| 1:XA:998(A):C:H2' | 1:XA:999:U:C6 | 2.56 | 0.40 |
| 9:XI:50:LEU:HD11 | 9:XI:81:ILE:HG21 | 2.02 | 0.40 |
| 16:XP:6:LEU:HD13 | 16:XP:6:LEU:HA | 1.96 | 0.40 |
| 17:XQ:40:LYS:HB2 | 17:XQ:40:LYS:HE2 | 1.88 | 0.40 |
| 19:XS:85:LYS:HA | 19:XS:85:LYS:HD2 | 1.90 | 0.40 |
| 24:YA:1683:C:H2' | 24:YA:1684:C:H6 | 1.86 | 0.40 |
| 24:YA:730:C:H2' | 24:YA:731:C:H6 | 1.86 | 0.40 |
| 28:YF:28:ILE:HD13 | 28:YF:116:ASP:HB2 | 2.03 | 0.40 |
| 29:YG:55:LYS:O | 29:YG:58:GLN:HG3 | 2.21 | 0.40 |
| 32:YN:118:LYS:HA | 32:YN:118:LYS:HD2 | 1.78 | 0.40 |
| 43:YY:13:VAL:HG12 | 43:YY:74:PRO:HA | 2.02 | 0.40 |
| 1:QA:1268:A:H2' | 1:QA:1269:A:C8 | 2.56 | 0.40 |
| 1:QA:1422:G:H2' | 1:QA:1423:G:H8 | 1.87 | 0.40 |
| 16:QP:8:ARG:HA | 16:QP:17:TYR:HD1 | 1.86 | 0.40 |
| 1:QA:279:A:OP2 | 17:QQ:91:ARG:NH2 | 2.54 | 0.40 |
| 1:QA:324:G:P | 20:QT:22:ARG:HE | 2.45 | 0.40 |
| 24:RA:1295:C:H2' | 24:RA:1296:G:C8 | 2.57 | 0.40 |
| 24:RA:150:C:H2' | 24:RA:151:C:H6 | 1.87 | 0.40 |
| 24:RA:2188:C:H2' | 24:RA:2189:U:O4' | 2.21 | 0.40 |
| 31:RI:76:THR:OG1 | 31:RI:139:GLN:NE2 | 2.49 | 0.40 |
| 1:XA:1255:G:O2' | 1:XA:1258:G:N3 | 2.37 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:1303:C:H2' | 1:XA:1304:G:O4' | 2.21 | 0.40 |
| 1:XA:1342:C:H2' | 1:XA:1343:G:H8 | 1.84 | 0.40 |
| 13:XM:65:LYS:HB3 | 49:Y4:50:VAL:HG21 | 2.02 | 0.40 |
| 6:XF:50:TYR:OH | 18:XR:75:ILE:O | 2.40 | 0.40 |
| 1:XA:1320:C:O2 | 19:XS:36:ARG:NH2 | 2.54 | 0.40 |
| 1:XA:323:U:O2' | 20:XT:22:ARG:HD3 | 2.21 | 0.40 |
| 22:XV:4:U:O2' | 22:XV:5:G:H8 | 2.04 | 0.40 |
| 48:Y3:28:LEU:HD22 | 48:Y3:35:ARG:HD3 | 2.02 | 0.40 |
| 54:Y9:6:SER:O | 54:Y9:6:SER:OG | 2.32 | 0.40 |
| 24:YA:1203:G:H1' | 24:YA:1242:A:N6 | 2.36 | 0.40 |
| 24:YA:1345:C:H2' | 24:YA:1346:G:H8 | 1.87 | 0.40 |
| 24:YA:1604:C:O2' | 24:YA:1610:A:N1 | 2.46 | 0.40 |
| 24:YA:186:G:H2' | 24:YA:187:G:C8 | 2.56 | 0.40 |
| 24:YA:1907:G:O6 | 24:YA:1924:C:N4 | 2.55 | 0.40 |
| 24:YA:1947:C:H2' | 24:YA:1948:G:H8 | 1.85 | 0.40 |
| 24:YA:1952:A:N3 | 24:YA:2560:C:O2' | 2.43 | 0.40 |
| 24:YA:1990:C:H2' | 24:YA:1991:U:C6 | 2.56 | 0.40 |
| 24:YA:2243:U:H2' | 24:YA:2244:U:C6 | 2.56 | 0.40 |
| 24:YA:2354:G:H4' | 45:Y0:35:ASN:ND2 | 2.36 | 0.40 |
| 24:YA:2626:C:H2' | 24:YA:2627:G:C8 | 2.51 | 0.40 |
| 24:YA:2661:G:H2' | 24:YA:2662:A:C8 | 2.56 | 0.40 |
| 24:YA:2698:U:H2' | 24:YA:2699:C:H6 | 1.87 | 0.40 |
| 24:YA:27:G:N2 | 24:YA:513:A:OP2 | 2.54 | 0.40 |
| 24:YA:864:G:H2' | 24:YA:865:C:C6 | 2.57 | 0.40 |
| 24:YA:2637:U:H5'' | 27:YE:82:ARG:NH1 | 2.35 | 0.40 |
| 44:YZ:48:PHE:HA | 44:YZ:51:ALA:HB3 | 2.02 | 0.40 |
| 1:QA:1298:C:H4' | 1:QA:1299:A:C5 | 2.57 | 0.40 |
| 1:QA:1346:A:H1' | 1:QA:1347:G:OP2 | 2.22 | 0.40 |
| 1:QA:173:U:H5'' | 1:QA:197:A:O4' | 2.21 | 0.40 |
| 1:QA:448:A:OP2 | 1:QA:485:G:N2 | 2.25 | 0.40 |
| 1:QA:538:G:H2' | 1:QA:539:A:C8 | 2.56 | 0.40 |
| 3:QC:8:ILE:HD12 | 3:QC:16:ARG:NH1 | 2.36 | 0.40 |
| 3:QC:152:ILE:HG12 | 3:QC:199:LYS:HB3 | 2.03 | 0.40 |
| 3:QC:30:ARG:O | 3:QC:34:LEU:HD12 | 2.21 | 0.40 |
| 5:QE:121:LYS:HA | 5:QE:121:LYS:HD2 | 1.83 | 0.40 |
| 12:QL:55:VAL:HG12 | 12:QL:69:TYR:HA | 2.04 | 0.40 |
| 20:QT:26:ASN:HB2 | 20:QT:71:THR:HG23 | 2.02 | 0.40 |
| 53:R8:26:LYS:HD2 | 53:R8:26:LYS:HA | 1.89 | 0.40 |
| 24:RA:137(A):G:O6 | 24:RA:139:G:O2' | 2.34 | 0.40 |
| 24:RA:1823:G:H2' | 24:RA:1824:G:H8 | 1.86 | 0.40 |
| 24:RA:829:A:N7 | 24:RA:2248:C:H5' | 2.37 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:RA:2315:G:H2' | 24:RA:2316:C:C6 | 2.55 | 0.40 |
| 24:RA:2287:A:H62 | 24:RA:2344:U:H3 | 1.70 | 0.40 |
| 24:RA:2377:A:H2' | 24:RA:2378:A:C8 | 2.55 | 0.40 |
| 24:RA:376:C:H2' | 24:RA:377:C:C6 | 2.56 | 0.40 |
| 24:RA:691:C:H2' | 24:RA:692:C:H6 | 1.86 | 0.40 |
| 27:RE:116:VAL:HG11 | 27:RE:138:PRO:HD3 | 2.03 | 0.40 |
| 27:RE:114:ALA:HB3 | 27:RE:160:TYR:HB3 | 2.02 | 0.40 |
| 32:RN:114:ARG:H | 32:RN:114:ARG:HG2 | 1.66 | 0.40 |
| 34:RP:79:ARG:HD3 | 34:RP:79:ARG:HA | 1.95 | 0.40 |
| 37:RS:96:GLY:H | 37:RS:99:LYS:HE3 | 1.87 | 0.40 |
| 1:XA:1322:C:O2' | 1:XA:1323:G:OP2 | 2.38 | 0.40 |
| 1:XA:165:C:H2' | 1:XA:166:G:C8 | 2.56 | 0.40 |
| 1:XA:636:U:H2' | 1:XA:637:G:C8 | 2.56 | 0.40 |
| 1:XA:79:G:H2' | 1:XA:80:G:H8 | 1.85 | 0.40 |
| 1:XA:822:C:H2' | 1:XA:823:G:C8 | 2.56 | 0.40 |
| 5:XE:43:LEU:HD12 | 5:XE:43:LEU:HA | 1.81 | 0.40 |
| 14:XN:15:LYS:HD3 | 14:XN:15:LYS:HA | 1.89 | 0.40 |
| 16:XP:71:ARG:HH12 | 16:XP:75:ARG:CZ | 2.34 | 0.40 |
| 20:XT:51:GLU:O | 20:XT:55:ILE:HG12 | 2.21 | 0.40 |
| 24:YA:1541:U:H2' | 24:YA:1542:G:O4' | 2.22 | 0.40 |
| 24:YA:1629:U:H2' | 24:YA:1630:G:H8 | 1.86 | 0.40 |
| 24:YA:1658:C:H2' | 24:YA:1659:U:C6 | 2.57 | 0.40 |
| 24:YA:184:C:H2' | 24:YA:185:U:C6 | 2.56 | 0.40 |
| 24:YA:2257:U:H2' | 24:YA:2258:C:C6 | 2.56 | 0.40 |
| 24:YA:230:U:H2' | 24:YA:231:C:H6 | 1.86 | 0.40 |
| 28:YF:152:GLU:O | 28:YF:154:VAL:HG23 | 2.21 | 0.40 |
| 30:YH:9:ILE:HA | 30:YH:10:PRO:HD3 | 1.89 | 0.40 |
| 1:QA:1137:C:O2' | 1:QA:1138:G:H5'' | 2.21 | 0.40 |
| 1:QA:1308:U:H2' | 1:QA:1309:G:C8 | 2.57 | 0.40 |
| 1:QA:224:C:H2' | 1:QA:225:C:H6 | 1.86 | 0.40 |
| 1:QA:900:A:H2' | 1:QA:901:A:C8 | 2.56 | 0.40 |
| 1:QA:947:G:O3' | 13:QM:109:THR:OG1 | 2.38 | 0.40 |
| 3:QC:90:GLU:O | 3:QC:93:LYS:NZ | 2.52 | 0.40 |
| 4:QD:201:GLN:HA | 4:QD:204:ILE:HD12 | 2.03 | 0.40 |
| 5:QE:5:ASP:OD1 | 5:QE:5:ASP:N | 2.55 | 0.40 |
| 13:QM:52:GLU:O | 13:QM:56:LEU:HB2 | 2.22 | 0.40 |
| 24:RA:1119:C:H2' | 24:RA:1120:G:H8 | 1.86 | 0.40 |
| 24:RA:1165:U:H2' | 24:RA:1166:C:C6 | 2.56 | 0.40 |
| 24:RA:1670:C:H2' | 24:RA:1671:U:O4' | 2.21 | 0.40 |
| 24:RA:2019:A:N7 | 50:R5:9:LYS:NZ | 2.61 | 0.40 |
| 24:RA:2074:U:H2' | 24:RA:2075:U:C6 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:RA:2231:C:H2' | 24:RA:2232:U:O4' | 2.21 | 0.40 |
| 24:RA:2303:G:O2' | 29:RG:132:ASN:HB2 | 2.20 | 0.40 |
| 24:RA:404:C:H1' | 24:RA:405:U:OP2 | 2.21 | 0.40 |
| 24:RA:479:A:OP1 | 43:RY:34:LYS:NZ | 2.42 | 0.40 |
| 25:RB:66:A:H61 | 25:RB:107:U:H2' | 1.86 | 0.40 |
| 26:RD:36:PRO:HA | 26:RD:62:TYR:O | 2.22 | 0.40 |
| 27:RE:6:GLY:HA2 | 27:RE:51:PHE:CZ | 2.57 | 0.40 |
| 38:RT:22:PHE:HA | 38:RT:91:ARG:HH12 | 1.86 | 0.40 |
| 1:XA:1006:C:H2' | 1:XA:1007:C:C6 | 2.57 | 0.40 |
| 1:XA:1304:G:N2 | 1:XA:1333:A:H62 | 2.19 | 0.40 |
| 1:XA:1431:C:H2' | 1:XA:1432:G:O4' | 2.20 | 0.40 |
| 1:XA:338:A:H2' | 1:XA:339:C:C6 | 2.57 | 0.40 |
| 1:XA:993:G:H2' | 1:XA:995:C:H41 | 1.85 | 0.40 |
| 7:XG:20:ASP:OD1 | 7:XG:21:VAL:N | 2.54 | 0.40 |
| 13:XM:40:ASN:HA | 13:XM:41:PRO:HD3 | 1.96 | 0.40 |
| 13:XM:76:ALA:O | 13:XM:80:ARG:HG2 | 2.22 | 0.40 |
| 22:XV:73:G:H2' | 22:XV:74:A:C8 | 2.56 | 0.40 |
| 24:YA:2230:G:O2' | 46:Y1:43:TYR:O | 2.27 | 0.40 |
| 51:Y6:9:LEU:HD13 | 51:Y6:51:GLU:HB2 | 2.04 | 0.40 |
| 53:Y8:3:LYS:HG3 | 53:Y8:3:LYS:H | 1.68 | 0.40 |
| 24:YA:1165:U:H2' | 24:YA:1166:C:H6 | 1.87 | 0.40 |
| 24:YA:2031:A:N3 | 24:YA:2455:G:O2' | 2.51 | 0.40 |
| 24:YA:2055:C:H4' | 24:YA:2056:G:H5'' | 2.04 | 0.40 |
| 24:YA:610:C:H2' | 24:YA:611:C:H6 | 1.85 | 0.40 |
| 24:YA:658:C:H2' | 24:YA:659:C:C6 | 2.56 | 0.40 |
| 24:YA:664:C:H2' | 24:YA:665:C:H6 | 1.87 | 0.40 |
| 24:YA:667:U:H2' | 24:YA:668:G:O4' | 2.21 | 0.40 |
| 24:YA:1656:C:P | 27:YE:136:ARG:HE | 2.44 | 0.40 |
| 29:YG:106:LEU:HA | 29:YG:110:ALA:HB3 | 2.03 | 0.40 |
| 29:YG:124:SER:HB2 | 29:YG:131:TYR:CE1 | 2.57 | 0.40 |
| 29:YG:83:ARG:HG3 | 29:YG:84:LYS:H | 1.85 | 0.40 |
| 34:YP:107:LYS:O | 34:YP:109:GLY:N | 2.55 | 0.40 |
| 35:YQ:5:ARG:HE | 35:YQ:6:ARG:H | 1.68 | 0.40 |
| 38:YT:107:ASP:O | 38:YT:110:ILE:HG12 | 2.21 | 0.40 |
| 42:YX:21:PHE:HA | 42:YX:26:TYR:HE1 | 1.86 | 0.40 |

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------------|--------------------------|-------------------|
| 40:YV:53:GLU:CB | 50:Y5:59:GLU:OE1[4_445] | 1.95 | 0.25 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------------|--------------------------|-------------------|
| 11:QK:99:GLN:OE1 | 3:XC:79:ARG:CD[4_555] | 2.01 | 0.19 |
| 24:RA:2137:C:OP1 | 1:XA:999:U:O2'[4_555] | 2.05 | 0.15 |
| 30:YH:46:GLU:OE2 | 43:YY:23:ARG:NH1[4_445] | 2.08 | 0.12 |
| 24:RA:306:U:O3' | 47:Y2:17:SER:OG[3_555] | 2.12 | 0.08 |
| 24:RA:307:G:O3' | 47:Y2:15:LYS:NZ[3_555] | 2.13 | 0.07 |
| 24:RA:2217:G:OP1 | 4:XD:159:ARG:NH2[4_555] | 2.14 | 0.06 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | QB | 233/256 (91%) | 204 (88%) | 27 (12%) | 2 (1%) | 17 | 54 |
| 2 | XB | 234/256 (91%) | 207 (88%) | 27 (12%) | 0 | 100 | 100 |
| 3 | QC | 203/239 (85%) | 189 (93%) | 13 (6%) | 1 (0%) | 29 | 66 |
| 3 | XC | 203/239 (85%) | 184 (91%) | 18 (9%) | 1 (0%) | 29 | 66 |
| 4 | QD | 206/209 (99%) | 188 (91%) | 18 (9%) | 0 | 100 | 100 |
| 4 | XD | 206/209 (99%) | 191 (93%) | 15 (7%) | 0 | 100 | 100 |
| 5 | QE | 149/162 (92%) | 139 (93%) | 9 (6%) | 1 (1%) | 22 | 60 |
| 5 | XE | 149/162 (92%) | 138 (93%) | 11 (7%) | 0 | 100 | 100 |
| 6 | QF | 99/101 (98%) | 95 (96%) | 4 (4%) | 0 | 100 | 100 |
| 6 | XF | 99/101 (98%) | 98 (99%) | 1 (1%) | 0 | 100 | 100 |
| 7 | QG | 153/156 (98%) | 145 (95%) | 8 (5%) | 0 | 100 | 100 |
| 7 | XG | 153/156 (98%) | 148 (97%) | 5 (3%) | 0 | 100 | 100 |
| 8 | QH | 135/138 (98%) | 126 (93%) | 9 (7%) | 0 | 100 | 100 |
| 8 | XH | 135/138 (98%) | 128 (95%) | 7 (5%) | 0 | 100 | 100 |
| 9 | QI | 123/128 (96%) | 113 (92%) | 9 (7%) | 1 (1%) | 19 | 57 |
| 9 | XI | 124/128 (97%) | 116 (94%) | 8 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 10 | QJ | 97/105 (92%) | 93 (96%) | 4 (4%) | 0 | 100 | 100 |
| 10 | XJ | 94/105 (90%) | 83 (88%) | 11 (12%) | 0 | 100 | 100 |
| 11 | QK | 117/129 (91%) | 111 (95%) | 6 (5%) | 0 | 100 | 100 |
| 11 | XK | 114/129 (88%) | 110 (96%) | 4 (4%) | 0 | 100 | 100 |
| 12 | QL | 123/132 (93%) | 111 (90%) | 11 (9%) | 1 (1%) | 19 | 57 |
| 12 | XL | 120/132 (91%) | 104 (87%) | 15 (12%) | 1 (1%) | 19 | 57 |
| 13 | QM | 118/126 (94%) | 102 (86%) | 15 (13%) | 1 (1%) | 19 | 57 |
| 13 | XM | 117/126 (93%) | 99 (85%) | 17 (14%) | 1 (1%) | 17 | 54 |
| 14 | QN | 58/61 (95%) | 51 (88%) | 6 (10%) | 1 (2%) | 9 | 42 |
| 14 | XN | 58/61 (95%) | 52 (90%) | 5 (9%) | 1 (2%) | 9 | 42 |
| 15 | QO | 86/89 (97%) | 82 (95%) | 4 (5%) | 0 | 100 | 100 |
| 15 | XO | 85/89 (96%) | 84 (99%) | 1 (1%) | 0 | 100 | 100 |
| 16 | QP | 82/88 (93%) | 79 (96%) | 3 (4%) | 0 | 100 | 100 |
| 16 | XP | 82/88 (93%) | 81 (99%) | 1 (1%) | 0 | 100 | 100 |
| 17 | QQ | 98/105 (93%) | 93 (95%) | 5 (5%) | 0 | 100 | 100 |
| 17 | XQ | 98/105 (93%) | 95 (97%) | 3 (3%) | 0 | 100 | 100 |
| 18 | QR | 68/88 (77%) | 66 (97%) | 2 (3%) | 0 | 100 | 100 |
| 18 | XR | 68/88 (77%) | 62 (91%) | 6 (9%) | 0 | 100 | 100 |
| 19 | QS | 81/93 (87%) | 73 (90%) | 8 (10%) | 0 | 100 | 100 |
| 19 | XS | 82/93 (88%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 20 | QT | 97/106 (92%) | 91 (94%) | 6 (6%) | 0 | 100 | 100 |
| 20 | XT | 97/106 (92%) | 90 (93%) | 6 (6%) | 1 (1%) | 15 | 52 |
| 21 | QU | 23/27 (85%) | 20 (87%) | 3 (13%) | 0 | 100 | 100 |
| 21 | XU | 23/27 (85%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 26 | RD | 270/276 (98%) | 245 (91%) | 23 (8%) | 2 (1%) | 22 | 60 |
| 26 | YD | 270/276 (98%) | 248 (92%) | 20 (7%) | 2 (1%) | 22 | 60 |
| 27 | RE | 203/206 (98%) | 170 (84%) | 31 (15%) | 2 (1%) | 15 | 52 |
| 27 | YE | 203/206 (98%) | 166 (82%) | 35 (17%) | 2 (1%) | 15 | 52 |
| 28 | RF | 200/210 (95%) | 189 (94%) | 11 (6%) | 0 | 100 | 100 |
| 28 | YF | 200/210 (95%) | 189 (94%) | 11 (6%) | 0 | 100 | 100 |
| 29 | RG | 179/182 (98%) | 148 (83%) | 29 (16%) | 2 (1%) | 14 | 50 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 29 | YG | 179/182 (98%) | 150 (84%) | 27 (15%) | 2 (1%) | 14 | 50 |
| 30 | RH | 172/180 (96%) | 147 (86%) | 20 (12%) | 5 (3%) | 4 | 32 |
| 30 | YH | 172/180 (96%) | 150 (87%) | 18 (10%) | 4 (2%) | 6 | 37 |
| 31 | RI | 144/148 (97%) | 121 (84%) | 20 (14%) | 3 (2%) | 7 | 38 |
| 31 | YI | 144/148 (97%) | 120 (83%) | 21 (15%) | 3 (2%) | 7 | 38 |
| 32 | RN | 136/140 (97%) | 120 (88%) | 15 (11%) | 1 (1%) | 22 | 60 |
| 32 | YN | 136/140 (97%) | 119 (88%) | 17 (12%) | 0 | 100 | 100 |
| 33 | RO | 120/122 (98%) | 112 (93%) | 8 (7%) | 0 | 100 | 100 |
| 33 | YO | 120/122 (98%) | 112 (93%) | 8 (7%) | 0 | 100 | 100 |
| 34 | RP | 148/150 (99%) | 120 (81%) | 26 (18%) | 2 (1%) | 11 | 45 |
| 34 | YP | 145/150 (97%) | 119 (82%) | 25 (17%) | 1 (1%) | 22 | 60 |
| 35 | RQ | 139/141 (99%) | 119 (86%) | 19 (14%) | 1 (1%) | 22 | 60 |
| 35 | YQ | 139/141 (99%) | 117 (84%) | 21 (15%) | 1 (1%) | 22 | 60 |
| 36 | RR | 115/118 (98%) | 108 (94%) | 5 (4%) | 2 (2%) | 9 | 42 |
| 36 | YR | 115/118 (98%) | 107 (93%) | 7 (6%) | 1 (1%) | 17 | 54 |
| 37 | RS | 109/112 (97%) | 93 (85%) | 15 (14%) | 1 (1%) | 17 | 54 |
| 37 | YS | 109/112 (97%) | 92 (84%) | 17 (16%) | 0 | 100 | 100 |
| 38 | RT | 135/146 (92%) | 118 (87%) | 15 (11%) | 2 (2%) | 10 | 45 |
| 38 | YT | 135/146 (92%) | 114 (84%) | 19 (14%) | 2 (2%) | 10 | 45 |
| 39 | RU | 115/118 (98%) | 107 (93%) | 7 (6%) | 1 (1%) | 17 | 54 |
| 39 | YU | 115/118 (98%) | 106 (92%) | 8 (7%) | 1 (1%) | 17 | 54 |
| 40 | RV | 99/101 (98%) | 87 (88%) | 11 (11%) | 1 (1%) | 15 | 52 |
| 40 | YV | 99/101 (98%) | 86 (87%) | 12 (12%) | 1 (1%) | 15 | 52 |
| 41 | RW | 111/113 (98%) | 105 (95%) | 5 (4%) | 1 (1%) | 17 | 54 |
| 41 | YW | 111/113 (98%) | 101 (91%) | 9 (8%) | 1 (1%) | 17 | 54 |
| 42 | RX | 90/96 (94%) | 89 (99%) | 1 (1%) | 0 | 100 | 100 |
| 42 | YX | 90/96 (94%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 43 | RY | 105/110 (96%) | 101 (96%) | 4 (4%) | 0 | 100 | 100 |
| 43 | YY | 105/110 (96%) | 99 (94%) | 6 (6%) | 0 | 100 | 100 |
| 44 | RZ | 181/206 (88%) | 146 (81%) | 32 (18%) | 3 (2%) | 9 | 42 |
| 44 | YZ | 181/206 (88%) | 149 (82%) | 29 (16%) | 3 (2%) | 9 | 42 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 45 | R0 | 79/85 (93%) | 74 (94%) | 5 (6%) | 0 | 100 | 100 |
| 45 | Y0 | 72/85 (85%) | 69 (96%) | 3 (4%) | 0 | 100 | 100 |
| 46 | R1 | 95/98 (97%) | 86 (90%) | 9 (10%) | 0 | 100 | 100 |
| 46 | Y1 | 91/98 (93%) | 83 (91%) | 8 (9%) | 0 | 100 | 100 |
| 47 | R2 | 67/72 (93%) | 63 (94%) | 3 (4%) | 1 (2%) | 10 | 45 |
| 47 | Y2 | 67/72 (93%) | 63 (94%) | 3 (4%) | 1 (2%) | 10 | 45 |
| 48 | R3 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 48 | Y3 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 49 | R4 | 67/71 (94%) | 53 (79%) | 13 (19%) | 1 (2%) | 10 | 45 |
| 49 | Y4 | 67/71 (94%) | 53 (79%) | 13 (19%) | 1 (2%) | 10 | 45 |
| 50 | R5 | 57/60 (95%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 50 | Y5 | 57/60 (95%) | 52 (91%) | 5 (9%) | 0 | 100 | 100 |
| 51 | R6 | 51/54 (94%) | 51 (100%) | 0 | 0 | 100 | 100 |
| 51 | Y6 | 51/54 (94%) | 47 (92%) | 4 (8%) | 0 | 100 | 100 |
| 52 | R7 | 45/49 (92%) | 45 (100%) | 0 | 0 | 100 | 100 |
| 52 | Y7 | 46/49 (94%) | 45 (98%) | 1 (2%) | 0 | 100 | 100 |
| 53 | R8 | 62/65 (95%) | 48 (77%) | 11 (18%) | 3 (5%) | 2 | 23 |
| 53 | Y8 | 62/65 (95%) | 47 (76%) | 13 (21%) | 2 (3%) | 4 | 31 |
| 54 | R9 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 54 | Y9 | 35/37 (95%) | 33 (94%) | 2 (6%) | 0 | 100 | 100 |
| All | All | 11449/12128 (94%) | 10319 (90%) | 1055 (9%) | 75 (1%) | 22 | 60 |

All (75) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | RE | 18 | ASP |
| 31 | RI | 15 | VAL |
| 38 | RT | 124 | ASP |
| 44 | RZ | 53 | ILE |
| 53 | R8 | 30 | ARG |
| 27 | YE | 18 | ASP |
| 30 | YH | 86 | GLU |
| 30 | YH | 152 | ARG |
| 31 | YI | 15 | VAL |
| 38 | YT | 123 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | YT | 124 | ASP |
| 44 | YZ | 53 | ILE |
| 53 | Y8 | 30 | ARG |
| 3 | QC | 12 | LEU |
| 14 | QN | 17 | LYS |
| 26 | RD | 243 | GLY |
| 34 | RP | 108 | LYS |
| 36 | RR | 3 | HIS |
| 38 | RT | 123 | GLN |
| 53 | R8 | 29 | LYS |
| 12 | XL | 105 | TYR |
| 14 | XN | 17 | LYS |
| 34 | YP | 108 | LYS |
| 53 | Y8 | 29 | LYS |
| 12 | QL | 46 | LYS |
| 27 | RE | 83 | ASP |
| 30 | RH | 86 | GLU |
| 30 | RH | 87 | LEU |
| 30 | RH | 152 | ARG |
| 31 | RI | 10 | GLU |
| 32 | RN | 22 | THR |
| 36 | RR | 4 | LEU |
| 37 | RS | 111 | GLU |
| 40 | RV | 44 | LYS |
| 41 | RW | 66 | GLU |
| 49 | R4 | 47 | GLN |
| 26 | YD | 243 | GLY |
| 27 | YE | 83 | ASP |
| 29 | YG | 81 | LYS |
| 39 | YU | 92 | ARG |
| 41 | YW | 66 | GLU |
| 49 | Y4 | 47 | GLN |
| 9 | QI | 107 | ARG |
| 13 | QM | 14 | ARG |
| 29 | RG | 81 | LYS |
| 39 | RU | 92 | ARG |
| 44 | RZ | 52 | SER |
| 47 | R2 | 70 | GLN |
| 29 | YG | 83 | ARG |
| 30 | YH | 87 | LEU |
| 35 | YQ | 78 | PRO |
| 47 | Y2 | 70 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | RG | 82 | LEU |
| 30 | RH | 12 | PRO |
| 35 | RQ | 78 | PRO |
| 3 | XC | 12 | LEU |
| 13 | XM | 13 | LYS |
| 30 | YH | 12 | PRO |
| 31 | YI | 123 | LEU |
| 36 | YR | 4 | LEU |
| 40 | YV | 44 | LYS |
| 44 | YZ | 52 | SER |
| 30 | RH | 129 | THR |
| 26 | YD | 36 | PRO |
| 53 | R8 | 53 | PRO |
| 26 | RD | 36 | PRO |
| 5 | QE | 74 | GLY |
| 34 | RP | 10 | PRO |
| 44 | RZ | 166 | SER |
| 2 | QB | 208 | ILE |
| 31 | RI | 16 | GLY |
| 31 | YI | 16 | GLY |
| 44 | YZ | 165 | VAL |
| 2 | QB | 232 | PRO |
| 20 | XT | 97 | ALA |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2 | QB | 203/220 (92%) | 200 (98%) | 3 (2%) | 65 | 79 |
| 2 | XB | 204/220 (93%) | 201 (98%) | 3 (2%) | 65 | 79 |
| 3 | QC | 159/188 (85%) | 154 (97%) | 5 (3%) | 40 | 63 |
| 3 | XC | 159/188 (85%) | 157 (99%) | 2 (1%) | 69 | 81 |
| 4 | QD | 180/181 (99%) | 176 (98%) | 4 (2%) | 52 | 71 |
| 4 | XD | 180/181 (99%) | 175 (97%) | 5 (3%) | 43 | 65 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 5 | QE | 116/123 (94%) | 115 (99%) | 1 (1%) | 78 | 87 |
| 5 | XE | 116/123 (94%) | 115 (99%) | 1 (1%) | 78 | 87 |
| 6 | QF | 90/90 (100%) | 90 (100%) | 0 | 100 | 100 |
| 6 | XF | 90/90 (100%) | 90 (100%) | 0 | 100 | 100 |
| 7 | QG | 126/127 (99%) | 122 (97%) | 4 (3%) | 39 | 62 |
| 7 | XG | 126/127 (99%) | 124 (98%) | 2 (2%) | 62 | 79 |
| 8 | QH | 118/119 (99%) | 116 (98%) | 2 (2%) | 60 | 78 |
| 8 | XH | 118/119 (99%) | 116 (98%) | 2 (2%) | 60 | 78 |
| 9 | QI | 96/99 (97%) | 94 (98%) | 2 (2%) | 53 | 72 |
| 9 | XI | 97/99 (98%) | 95 (98%) | 2 (2%) | 53 | 72 |
| 10 | QJ | 89/92 (97%) | 88 (99%) | 1 (1%) | 73 | 84 |
| 10 | XJ | 86/92 (94%) | 83 (96%) | 3 (4%) | 36 | 61 |
| 11 | QK | 90/99 (91%) | 89 (99%) | 1 (1%) | 73 | 84 |
| 11 | XK | 88/99 (89%) | 88 (100%) | 0 | 100 | 100 |
| 12 | QL | 104/109 (95%) | 103 (99%) | 1 (1%) | 76 | 85 |
| 12 | XL | 103/109 (94%) | 102 (99%) | 1 (1%) | 76 | 85 |
| 13 | QM | 96/101 (95%) | 93 (97%) | 3 (3%) | 40 | 63 |
| 13 | XM | 95/101 (94%) | 92 (97%) | 3 (3%) | 39 | 62 |
| 14 | QN | 49/50 (98%) | 47 (96%) | 2 (4%) | 30 | 57 |
| 14 | XN | 49/50 (98%) | 49 (100%) | 0 | 100 | 100 |
| 15 | QO | 79/80 (99%) | 79 (100%) | 0 | 100 | 100 |
| 15 | XO | 79/80 (99%) | 79 (100%) | 0 | 100 | 100 |
| 16 | QP | 72/74 (97%) | 72 (100%) | 0 | 100 | 100 |
| 16 | XP | 72/74 (97%) | 72 (100%) | 0 | 100 | 100 |
| 17 | QQ | 95/97 (98%) | 94 (99%) | 1 (1%) | 73 | 84 |
| 17 | XQ | 95/97 (98%) | 94 (99%) | 1 (1%) | 73 | 84 |
| 18 | QR | 61/77 (79%) | 61 (100%) | 0 | 100 | 100 |
| 18 | XR | 61/77 (79%) | 61 (100%) | 0 | 100 | 100 |
| 19 | QS | 72/80 (90%) | 71 (99%) | 1 (1%) | 67 | 80 |
| 19 | XS | 73/80 (91%) | 73 (100%) | 0 | 100 | 100 |
| 20 | QT | 76/82 (93%) | 75 (99%) | 1 (1%) | 69 | 81 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 20 | XT | 76/82 (93%) | 76 (100%) | 0 | 100 | 100 |
| 21 | QU | 20/22 (91%) | 19 (95%) | 1 (5%) | 24 | 52 |
| 21 | XU | 20/22 (91%) | 19 (95%) | 1 (5%) | 24 | 52 |
| 26 | RD | 214/218 (98%) | 212 (99%) | 2 (1%) | 78 | 87 |
| 26 | YD | 214/218 (98%) | 212 (99%) | 2 (1%) | 78 | 87 |
| 27 | RE | 165/166 (99%) | 164 (99%) | 1 (1%) | 86 | 91 |
| 27 | YE | 165/166 (99%) | 165 (100%) | 0 | 100 | 100 |
| 28 | RF | 161/166 (97%) | 161 (100%) | 0 | 100 | 100 |
| 28 | YF | 161/166 (97%) | 161 (100%) | 0 | 100 | 100 |
| 29 | RG | 155/156 (99%) | 154 (99%) | 1 (1%) | 86 | 91 |
| 29 | YG | 155/156 (99%) | 154 (99%) | 1 (1%) | 86 | 91 |
| 30 | RH | 145/148 (98%) | 144 (99%) | 1 (1%) | 84 | 90 |
| 30 | YH | 145/148 (98%) | 143 (99%) | 2 (1%) | 67 | 80 |
| 31 | RI | 122/124 (98%) | 122 (100%) | 0 | 100 | 100 |
| 31 | YI | 122/124 (98%) | 121 (99%) | 1 (1%) | 81 | 88 |
| 32 | RN | 117/119 (98%) | 117 (100%) | 0 | 100 | 100 |
| 32 | YN | 117/119 (98%) | 116 (99%) | 1 (1%) | 78 | 87 |
| 33 | RO | 100/100 (100%) | 100 (100%) | 0 | 100 | 100 |
| 33 | YO | 100/100 (100%) | 100 (100%) | 0 | 100 | 100 |
| 34 | RP | 116/116 (100%) | 114 (98%) | 2 (2%) | 60 | 78 |
| 34 | YP | 114/116 (98%) | 114 (100%) | 0 | 100 | 100 |
| 35 | RQ | 111/111 (100%) | 109 (98%) | 2 (2%) | 59 | 77 |
| 35 | YQ | 111/111 (100%) | 109 (98%) | 2 (2%) | 59 | 77 |
| 36 | RR | 100/101 (99%) | 100 (100%) | 0 | 100 | 100 |
| 36 | YR | 100/101 (99%) | 100 (100%) | 0 | 100 | 100 |
| 37 | RS | 87/88 (99%) | 86 (99%) | 1 (1%) | 73 | 84 |
| 37 | YS | 87/88 (99%) | 87 (100%) | 0 | 100 | 100 |
| 38 | RT | 120/127 (94%) | 119 (99%) | 1 (1%) | 81 | 88 |
| 38 | YT | 120/127 (94%) | 120 (100%) | 0 | 100 | 100 |
| 39 | RU | 93/94 (99%) | 92 (99%) | 1 (1%) | 73 | 84 |
| 39 | YU | 93/94 (99%) | 93 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 40 | RV | 82/82 (100%) | 81 (99%) | 1 (1%) | 71 | 83 |
| 40 | YV | 82/82 (100%) | 80 (98%) | 2 (2%) | 49 | 69 |
| 41 | RW | 92/92 (100%) | 92 (100%) | 0 | 100 | 100 |
| 41 | YW | 92/92 (100%) | 90 (98%) | 2 (2%) | 52 | 71 |
| 42 | RX | 74/78 (95%) | 74 (100%) | 0 | 100 | 100 |
| 42 | YX | 74/78 (95%) | 74 (100%) | 0 | 100 | 100 |
| 43 | RY | 88/91 (97%) | 87 (99%) | 1 (1%) | 73 | 84 |
| 43 | YY | 88/91 (97%) | 86 (98%) | 2 (2%) | 50 | 70 |
| 44 | RZ | 162/179 (90%) | 162 (100%) | 0 | 100 | 100 |
| 44 | YZ | 162/179 (90%) | 160 (99%) | 2 (1%) | 71 | 83 |
| 45 | R0 | 65/67 (97%) | 64 (98%) | 1 (2%) | 65 | 79 |
| 45 | Y0 | 60/67 (90%) | 59 (98%) | 1 (2%) | 60 | 78 |
| 46 | R1 | 82/83 (99%) | 81 (99%) | 1 (1%) | 71 | 83 |
| 46 | Y1 | 78/83 (94%) | 78 (100%) | 0 | 100 | 100 |
| 47 | R2 | 64/67 (96%) | 64 (100%) | 0 | 100 | 100 |
| 47 | Y2 | 64/67 (96%) | 64 (100%) | 0 | 100 | 100 |
| 48 | R3 | 51/52 (98%) | 50 (98%) | 1 (2%) | 55 | 73 |
| 48 | Y3 | 51/52 (98%) | 45 (88%) | 6 (12%) | 5 | 24 |
| 49 | R4 | 62/63 (98%) | 61 (98%) | 1 (2%) | 62 | 79 |
| 49 | Y4 | 62/63 (98%) | 60 (97%) | 2 (3%) | 39 | 62 |
| 50 | R5 | 51/52 (98%) | 51 (100%) | 0 | 100 | 100 |
| 50 | Y5 | 51/52 (98%) | 50 (98%) | 1 (2%) | 55 | 73 |
| 51 | R6 | 51/52 (98%) | 51 (100%) | 0 | 100 | 100 |
| 51 | Y6 | 51/52 (98%) | 50 (98%) | 1 (2%) | 55 | 73 |
| 52 | R7 | 40/42 (95%) | 40 (100%) | 0 | 100 | 100 |
| 52 | Y7 | 41/42 (98%) | 41 (100%) | 0 | 100 | 100 |
| 53 | R8 | 54/55 (98%) | 53 (98%) | 1 (2%) | 57 | 75 |
| 53 | Y8 | 54/55 (98%) | 54 (100%) | 0 | 100 | 100 |
| 54 | R9 | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 54 | Y9 | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| All | All | 9684/10066 (96%) | 9578 (99%) | 106 (1%) | 73 | 84 |

All (106) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | QB | 69 | LEU |
| 2 | QB | 133 | LYS |
| 2 | QB | 139 | LYS |
| 3 | QC | 21 | ARG |
| 3 | QC | 34 | LEU |
| 3 | QC | 110 | ASN |
| 3 | QC | 135 | LYS |
| 3 | QC | 190 | ARG |
| 4 | QD | 40 | PRO |
| 4 | QD | 46 | LYS |
| 4 | QD | 61 | LYS |
| 4 | QD | 131 | ARG |
| 5 | QE | 127 | ASN |
| 7 | QG | 29 | LYS |
| 7 | QG | 36 | LYS |
| 7 | QG | 94 | ARG |
| 7 | QG | 115 | ARG |
| 8 | QH | 122 | ARG |
| 8 | QH | 129 | VAL |
| 9 | QI | 28 | VAL |
| 9 | QI | 93 | ARG |
| 10 | QJ | 46 | ARG |
| 11 | QK | 123 | LYS |
| 12 | QL | 59 | ARG |
| 13 | QM | 20 | THR |
| 13 | QM | 66 | LEU |
| 13 | QM | 77 | ASN |
| 14 | QN | 9 | LYS |
| 14 | QN | 19 | ARG |
| 17 | QQ | 87 | LYS |
| 19 | QS | 67 | VAL |
| 20 | QT | 14 | LYS |
| 21 | QU | 10 | ARG |
| 26 | RD | 5 | LYS |
| 26 | RD | 36 | PRO |
| 27 | RE | 133 | LYS |
| 29 | RG | 33 | ARG |
| 30 | RH | 162 | ILE |
| 34 | RP | 45 | LEU |
| 34 | RP | 132 | LYS |
| 35 | RQ | 79 | LEU |
| 35 | RQ | 81 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37 | RS | 106 | ARG |
| 38 | RT | 112 | ARG |
| 39 | RU | 90 | VAL |
| 40 | RV | 50 | PRO |
| 43 | RY | 90 | LEU |
| 45 | R0 | 14 | ARG |
| 46 | R1 | 81 | LYS |
| 48 | R3 | 30 | ARG |
| 49 | R4 | 50 | VAL |
| 53 | R8 | 60 | LEU |
| 2 | XB | 64 | ARG |
| 2 | XB | 96 | ARG |
| 2 | XB | 145 | LEU |
| 3 | XC | 52 | LEU |
| 3 | XC | 130 | VAL |
| 4 | XD | 19 | LEU |
| 4 | XD | 132 | ARG |
| 4 | XD | 139 | ARG |
| 4 | XD | 141 | ARG |
| 4 | XD | 182 | LYS |
| 5 | XE | 24 | ARG |
| 7 | XG | 5 | ARG |
| 7 | XG | 94 | ARG |
| 8 | XH | 129 | VAL |
| 8 | XH | 135 | CYS |
| 9 | XI | 2 | GLU |
| 9 | XI | 110 | GLU |
| 10 | XJ | 5 | ARG |
| 10 | XJ | 46 | ARG |
| 10 | XJ | 60 | ARG |
| 12 | XL | 48 | PRO |
| 13 | XM | 31 | LYS |
| 13 | XM | 99 | ARG |
| 13 | XM | 102 | ARG |
| 17 | XQ | 100 | LYS |
| 21 | XU | 24 | ARG |
| 26 | YD | 36 | PRO |
| 26 | YD | 126 | GLN |
| 29 | YG | 33 | ARG |
| 30 | YH | 24 | VAL |
| 30 | YH | 69 | ARG |
| 31 | YI | 103 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | YN | 34 | LEU |
| 35 | YQ | 59 | ARG |
| 35 | YQ | 81 | VAL |
| 40 | YV | 20 | LEU |
| 40 | YV | 50 | PRO |
| 41 | YW | 17 | VAL |
| 41 | YW | 23 | LEU |
| 43 | YY | 21 | LYS |
| 43 | YY | 45 | VAL |
| 44 | YZ | 34 | ASN |
| 44 | YZ | 165 | VAL |
| 45 | Y0 | 14 | ARG |
| 48 | Y3 | 3 | ARG |
| 48 | Y3 | 4 | LEU |
| 48 | Y3 | 30 | ARG |
| 48 | Y3 | 37 | LEU |
| 48 | Y3 | 38 | GLU |
| 48 | Y3 | 44 | ARG |
| 49 | Y4 | 55 | ARG |
| 49 | Y4 | 62 | ARG |
| 50 | Y5 | 36 | CYS |
| 51 | Y6 | 15 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | QC | 98 | ASN |
| 3 | QC | 123 | GLN |
| 3 | QC | 170 | GLN |
| 9 | QI | 124 | GLN |
| 10 | QJ | 68 | HIS |
| 11 | QK | 99 | GLN |
| 47 | R2 | 9 | GLN |
| 2 | XB | 16 | HIS |
| 2 | XB | 95 | GLN |
| 6 | XF | 7 | ASN |
| 6 | XF | 32 | ASN |
| 13 | XM | 101 | GLN |
| 26 | YD | 115 | GLN |
| 26 | YD | 126 | GLN |
| 27 | YE | 66 | HIS |
| 28 | YF | 40 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | YG | 40 | ASN |
| 39 | YU | 94 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | QA | 1499/1521 (98%) | 271 (18%) | 37 (2%) |
| 1 | XA | 1498/1521 (98%) | 254 (16%) | 30 (2%) |
| 22 | QV | 76/77 (98%) | 15 (19%) | 1 (1%) |
| 22 | XV | 76/77 (98%) | 17 (22%) | 1 (1%) |
| 23 | QX | 18/19 (94%) | 5 (27%) | 2 (11%) |
| 23 | XX | 18/19 (94%) | 5 (27%) | 1 (5%) |
| 24 | RA | 2879/2915 (98%) | 571 (19%) | 41 (1%) |
| 24 | YA | 2880/2915 (98%) | 576 (20%) | 42 (1%) |
| 25 | RB | 119/122 (97%) | 18 (15%) | 1 (0%) |
| 25 | YB | 119/122 (97%) | 21 (17%) | 1 (0%) |
| All | All | 9182/9308 (98%) | 1753 (19%) | 157 (1%) |

All (1753) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | QA | 6 | G |
| 1 | QA | 9 | G |
| 1 | QA | 32 | A |
| 1 | QA | 39 | G |
| 1 | QA | 47 | C |
| 1 | QA | 48 | C |
| 1 | QA | 51 | A |
| 1 | QA | 64 | G |
| 1 | QA | 65 | U |
| 1 | QA | 66 | G |
| 1 | QA | 76 | G |
| 1 | QA | 90 | C |
| 1 | QA | 91 | C |
| 1 | QA | 95 | G |
| 1 | QA | 101 | A |
| 1 | QA | 108 | G |
| 1 | QA | 116 | A |
| 1 | QA | 120 | A |
| 1 | QA | 121 | C |
| 1 | QA | 129(A) | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | QA | 144 | G |
| 1 | QA | 146 | G |
| 1 | QA | 157 | G |
| 1 | QA | 158 | G |
| 1 | QA | 159 | G |
| 1 | QA | 162 | A |
| 1 | QA | 169 | C |
| 1 | QA | 173 | U |
| 1 | QA | 174 | C |
| 1 | QA | 182 | U |
| 1 | QA | 190 | G |
| 1 | QA | 191(A) | G |
| 1 | QA | 195 | A |
| 1 | QA | 197 | A |
| 1 | QA | 208 | U |
| 1 | QA | 209 | U |
| 1 | QA | 216 | G |
| 1 | QA | 244 | U |
| 1 | QA | 245 | C |
| 1 | QA | 247 | G |
| 1 | QA | 250 | A |
| 1 | QA | 251 | G |
| 1 | QA | 254 | G |
| 1 | QA | 262 | A |
| 1 | QA | 267 | C |
| 1 | QA | 270 | A |
| 1 | QA | 281 | G |
| 1 | QA | 289 | G |
| 1 | QA | 321 | A |
| 1 | QA | 328 | C |
| 1 | QA | 329 | A |
| 1 | QA | 332 | G |
| 1 | QA | 339 | C |
| 1 | QA | 343 | U |
| 1 | QA | 344 | A |
| 1 | QA | 346 | G |
| 1 | QA | 347 | G |
| 1 | QA | 348 | G |
| 1 | QA | 352 | C |
| 1 | QA | 353 | A |
| 1 | QA | 354 | G |
| 1 | QA | 356 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | QA | 367 | U |
| 1 | QA | 372 | C |
| 1 | QA | 373 | A |
| 1 | QA | 390 | C |
| 1 | QA | 397 | A |
| 1 | QA | 398 | C |
| 1 | QA | 411 | A |
| 1 | QA | 412 | A |
| 1 | QA | 413 | G |
| 1 | QA | 421 | U |
| 1 | QA | 422 | C |
| 1 | QA | 423 | G |
| 1 | QA | 424 | G |
| 1 | QA | 428 | G |
| 1 | QA | 429 | U |
| 1 | QA | 430 | A |
| 1 | QA | 442 | C |
| 1 | QA | 466 | C |
| 1 | QA | 482 | A |
| 1 | QA | 485 | G |
| 1 | QA | 486 | U |
| 1 | QA | 496 | A |
| 1 | QA | 497 | U |
| 1 | QA | 505 | G |
| 1 | QA | 509 | A |
| 1 | QA | 510 | A |
| 1 | QA | 511 | C |
| 1 | QA | 518 | C |
| 1 | QA | 521 | G |
| 1 | QA | 527 | G |
| 1 | QA | 532 | A |
| 1 | QA | 533 | A |
| 1 | QA | 545 | C |
| 1 | QA | 547 | A |
| 1 | QA | 559 | A |
| 1 | QA | 560 | U |
| 1 | QA | 565 | U |
| 1 | QA | 568 | G |
| 1 | QA | 572 | A |
| 1 | QA | 573 | A |
| 1 | QA | 576 | G |
| 1 | QA | 577 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | QA | 596 | C |
| 1 | QA | 618 | C |
| 1 | QA | 630 | G |
| 1 | QA | 631 | G |
| 1 | QA | 653 | A |
| 1 | QA | 665 | A |
| 1 | QA | 666 | G |
| 1 | QA | 686 | U |
| 1 | QA | 688 | G |
| 1 | QA | 701 | C |
| 1 | QA | 702 | A |
| 1 | QA | 703 | G |
| 1 | QA | 704 | A |
| 1 | QA | 722 | A |
| 1 | QA | 731 | G |
| 1 | QA | 748 | C |
| 1 | QA | 754 | C |
| 1 | QA | 755 | G |
| 1 | QA | 760 | G |
| 1 | QA | 777 | A |
| 1 | QA | 792 | A |
| 1 | QA | 793 | U |
| 1 | QA | 794 | A |
| 1 | QA | 813 | U |
| 1 | QA | 817 | C |
| 1 | QA | 819 | A |
| 1 | QA | 821 | G |
| 1 | QA | 828 | A |
| 1 | QA | 841 | U |
| 1 | QA | 842 | C |
| 1 | QA | 843 | U |
| 1 | QA | 848 | C |
| 1 | QA | 859 | A |
| 1 | QA | 871 | U |
| 1 | QA | 872 | A |
| 1 | QA | 873 | A |
| 1 | QA | 889 | A |
| 1 | QA | 891 | U |
| 1 | QA | 902 | G |
| 1 | QA | 914 | A |
| 1 | QA | 926 | G |
| 1 | QA | 927 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | QA | 934 | C |
| 1 | QA | 935 | A |
| 1 | QA | 960 | U |
| 1 | QA | 961 | U |
| 1 | QA | 968 | A |
| 1 | QA | 969 | A |
| 1 | QA | 971 | G |
| 1 | QA | 972 | C |
| 1 | QA | 974 | A |
| 1 | QA | 975 | A |
| 1 | QA | 976 | G |
| 1 | QA | 977 | A |
| 1 | QA | 982 | U |
| 1 | QA | 991 | U |
| 1 | QA | 992 | U |
| 1 | QA | 993 | G |
| 1 | QA | 994 | A |
| 1 | QA | 1001 | G |
| 1 | QA | 1004 | A |
| 1 | QA | 1006 | C |
| 1 | QA | 1009 | G |
| 1 | QA | 1020 | U |
| 1 | QA | 1024 | G |
| 1 | QA | 1025 | U |
| 1 | QA | 1028 | C |
| 1 | QA | 1029 | G |
| 1 | QA | 1030 | C |
| 1 | QA | 1031 | G |
| 1 | QA | 1032(A) | G |
| 1 | QA | 1033 | G |
| 1 | QA | 1034 | G |
| 1 | QA | 1042 | G |
| 1 | QA | 1054 | C |
| 1 | QA | 1064 | G |
| 1 | QA | 1065 | U |
| 1 | QA | 1066 | C |
| 1 | QA | 1080 | A |
| 1 | QA | 1081 | G |
| 1 | QA | 1082 | G |
| 1 | QA | 1094 | G |
| 1 | QA | 1095 | U |
| 1 | QA | 1101 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | QA | 1124 | G |
| 1 | QA | 1125 | U |
| 1 | QA | 1126 | U |
| 1 | QA | 1130 | A |
| 1 | QA | 1131 | G |
| 1 | QA | 1136 | U |
| 1 | QA | 1137 | C |
| 1 | QA | 1138 | G |
| 1 | QA | 1139 | G |
| 1 | QA | 1146 | A |
| 1 | QA | 1157 | A |
| 1 | QA | 1158 | C |
| 1 | QA | 1159 | U |
| 1 | QA | 1160 | G |
| 1 | QA | 1181 | G |
| 1 | QA | 1183 | A |
| 1 | QA | 1187 | G |
| 1 | QA | 1193 | G |
| 1 | QA | 1196 | U |
| 1 | QA | 1201 | A |
| 1 | QA | 1202 | G |
| 1 | QA | 1212 | U |
| 1 | QA | 1213 | A |
| 1 | QA | 1215 | G |
| 1 | QA | 1224 | G |
| 1 | QA | 1226 | C |
| 1 | QA | 1227 | A |
| 1 | QA | 1228 | C |
| 1 | QA | 1236 | A |
| 1 | QA | 1238 | A |
| 1 | QA | 1240 | U |
| 1 | QA | 1241 | G |
| 1 | QA | 1256 | A |
| 1 | QA | 1257 | U |
| 1 | QA | 1258 | G |
| 1 | QA | 1260 | C |
| 1 | QA | 1270 | C |
| 1 | QA | 1280 | A |
| 1 | QA | 1281 | U |
| 1 | QA | 1286 | A |
| 1 | QA | 1287 | A |
| 1 | QA | 1297 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | QA | 1298 | C |
| 1 | QA | 1299 | A |
| 1 | QA | 1301 | U |
| 1 | QA | 1302 | U |
| 1 | QA | 1303 | C |
| 1 | QA | 1305 | G |
| 1 | QA | 1320 | C |
| 1 | QA | 1321 | C |
| 1 | QA | 1322 | C |
| 1 | QA | 1323 | G |
| 1 | QA | 1331 | G |
| 1 | QA | 1334 | G |
| 1 | QA | 1335 | C |
| 1 | QA | 1336 | C |
| 1 | QA | 1337 | G |
| 1 | QA | 1346 | A |
| 1 | QA | 1347 | G |
| 1 | QA | 1348 | U |
| 1 | QA | 1353 | G |
| 1 | QA | 1362(A) | C |
| 1 | QA | 1364 | U |
| 1 | QA | 1397 | C |
| 1 | QA | 1398 | A |
| 1 | QA | 1419 | G |
| 1 | QA | 1442 | G |
| 1 | QA | 1446 | A |
| 1 | QA | 1447 | G |
| 1 | QA | 1452 | C |
| 1 | QA | 1453 | G |
| 1 | QA | 1492 | A |
| 1 | QA | 1494 | G |
| 1 | QA | 1499 | A |
| 1 | QA | 1502 | A |
| 1 | QA | 1504 | G |
| 1 | QA | 1506 | U |
| 1 | QA | 1517 | G |
| 1 | QA | 1520 | G |
| 1 | QA | 1527 | C |
| 1 | QA | 1528 | U |
| 1 | QA | 1529 | G |
| 1 | QA | 1530 | G |
| 22 | QV | 4 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | QV | 5 | G |
| 22 | QV | 8 | U |
| 22 | QV | 18 | U |
| 22 | QV | 19 | G |
| 22 | QV | 20 | G |
| 22 | QV | 22 | A |
| 22 | QV | 48 | U |
| 22 | QV | 49 | C |
| 22 | QV | 55 | U |
| 22 | QV | 64 | U |
| 22 | QV | 65 | C |
| 22 | QV | 68 | U |
| 22 | QV | 76 | C |
| 22 | QV | 77 | A |
| 23 | QX | 10 | G |
| 23 | QX | 14 | U |
| 23 | QX | 16 | A |
| 23 | QX | 21 | G |
| 23 | QX | 22 | G |
| 24 | RA | 10 | G |
| 24 | RA | 14 | A |
| 24 | RA | 15 | G |
| 24 | RA | 34 | C |
| 24 | RA | 46 | C |
| 24 | RA | 51 | G |
| 24 | RA | 55 | G |
| 24 | RA | 61 | G |
| 24 | RA | 72 | U |
| 24 | RA | 73 | A |
| 24 | RA | 74 | A |
| 24 | RA | 75 | G |
| 24 | RA | 82 | G |
| 24 | RA | 83 | G |
| 24 | RA | 101 | G |
| 24 | RA | 102 | G |
| 24 | RA | 103 | A |
| 24 | RA | 118 | A |
| 24 | RA | 120 | U |
| 24 | RA | 131 | G |
| 24 | RA | 140 | A |
| 24 | RA | 161 | U |
| 24 | RA | 177 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 24 | RA | 181 | A |
| 24 | RA | 188 | G |
| 24 | RA | 196 | A |
| 24 | RA | 199 | A |
| 24 | RA | 201 | C |
| 24 | RA | 214 | G |
| 24 | RA | 215 | G |
| 24 | RA | 216 | A |
| 24 | RA | 221 | A |
| 24 | RA | 222 | A |
| 24 | RA | 223 | A |
| 24 | RA | 229 | A |
| 24 | RA | 230 | U |
| 24 | RA | 233 | A |
| 24 | RA | 248 | G |
| 24 | RA | 249 | C |
| 24 | RA | 252 | G |
| 24 | RA | 265 | A |
| 24 | RA | 266 | G |
| 24 | RA | 270(L) | U |
| 24 | RA | 270(M) | U |
| 24 | RA | 270(N) | G |
| 24 | RA | 270(P) | C |
| 24 | RA | 270(Y) | G |
| 24 | RA | 271(C) | U |
| 24 | RA | 273(F) | C |
| 24 | RA | 275 | G |
| 24 | RA | 276 | A |
| 24 | RA | 277 | C |
| 24 | RA | 283 | A |
| 24 | RA | 294 | A |
| 24 | RA | 298 | G |
| 24 | RA | 299 | A |
| 24 | RA | 308 | G |
| 24 | RA | 309 | G |
| 24 | RA | 311 | A |
| 24 | RA | 312 | G |
| 24 | RA | 323 | G |
| 24 | RA | 324 | A |
| 24 | RA | 329 | G |
| 24 | RA | 330 | A |
| 24 | RA | 342 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 24 | RA | 346 | A |
| 24 | RA | 352 | G |
| 24 | RA | 363(F) | A |
| 24 | RA | 364 | C |
| 24 | RA | 371 | A |
| 24 | RA | 372 | G |
| 24 | RA | 373 | U |
| 24 | RA | 386 | G |
| 24 | RA | 395 | U |
| 24 | RA | 405 | U |
| 24 | RA | 406 | G |
| 24 | RA | 407 | G |
| 24 | RA | 411 | G |
| 24 | RA | 412 | A |
| 24 | RA | 428 | A |
| 24 | RA | 444 | C |
| 24 | RA | 448 | U |
| 24 | RA | 451 | C |
| 24 | RA | 452 | G |
| 24 | RA | 455 | C |
| 24 | RA | 456 | C |
| 24 | RA | 457 | A |
| 24 | RA | 470 | A |
| 24 | RA | 481 | G |
| 24 | RA | 504 | U |
| 24 | RA | 505 | A |
| 24 | RA | 509 | C |
| 24 | RA | 513 | A |
| 24 | RA | 527 | C |
| 24 | RA | 531 | C |
| 24 | RA | 532 | A |
| 24 | RA | 533 | G |
| 24 | RA | 537 | C |
| 24 | RA | 539 | G |
| 24 | RA | 540 | G |
| 24 | RA | 541 | C |
| 24 | RA | 546 | C |
| 24 | RA | 547 | A |
| 24 | RA | 563 | G |
| 24 | RA | 573 | G |
| 24 | RA | 574 | C |
| 24 | RA | 575 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 24 | RA | 583 | G |
| 24 | RA | 588 | U |
| 24 | RA | 603 | A |
| 24 | RA | 607 | U |
| 24 | RA | 614 | U |
| 24 | RA | 615 | G |
| 24 | RA | 617 | G |
| 24 | RA | 621 | A |
| 24 | RA | 627 | A |
| 24 | RA | 631 | A |
| 24 | RA | 637 | A |
| 24 | RA | 638 | G |
| 24 | RA | 645 | C |
| 24 | RA | 646 | A |
| 24 | RA | 647 | G |
| 24 | RA | 651 | G |
| 24 | RA | 652 | C |
| 24 | RA | 654 | A |
| 24 | RA | 654(A) | G |
| 24 | RA | 669 | G |
| 24 | RA | 686 | G |
| 24 | RA | 708 | C |
| 24 | RA | 717 | G |
| 24 | RA | 722 | A |
| 24 | RA | 726 | G |
| 24 | RA | 730 | C |
| 24 | RA | 731 | C |
| 24 | RA | 753 | C |
| 24 | RA | 761 | A |
| 24 | RA | 775 | G |
| 24 | RA | 776 | G |
| 24 | RA | 782 | A |
| 24 | RA | 783 | A |
| 24 | RA | 784 | A |
| 24 | RA | 785 | G |
| 24 | RA | 788 | A |
| 24 | RA | 790 | C |
| 24 | RA | 791 | C |
| 24 | RA | 792 | G |
| 24 | RA | 805 | G |
| 24 | RA | 811 | U |
| 24 | RA | 812 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 24 | RA | 819 | A |
| 24 | RA | 827 | U |
| 24 | RA | 828 | U |
| 24 | RA | 831 | G |
| 24 | RA | 847 | U |
| 24 | RA | 856 | C |
| 24 | RA | 857 | C |
| 24 | RA | 859 | G |
| 24 | RA | 869 | G |
| 24 | RA | 882 | G |
| 24 | RA | 884 | C |
| 24 | RA | 885 | C |
| 24 | RA | 886 | C |
| 24 | RA | 888 | C |
| 24 | RA | 889 | C |
| 24 | RA | 893 | C |
| 24 | RA | 896 | A |
| 24 | RA | 897 | C |
| 24 | RA | 900 | A |
| 24 | RA | 901 | A |
| 24 | RA | 907 | U |
| 24 | RA | 910 | A |
| 24 | RA | 914 | C |
| 24 | RA | 915 | C |
| 24 | RA | 917 | A |
| 24 | RA | 932 | G |
| 24 | RA | 941 | A |
| 24 | RA | 945 | A |
| 24 | RA | 946 | G |
| 24 | RA | 957 | A |
| 24 | RA | 959 | A |
| 24 | RA | 961 | C |
| 24 | RA | 973 | A |
| 24 | RA | 974 | G |
| 24 | RA | 974(A) | C |
| 24 | RA | 980 | A |
| 24 | RA | 983 | A |
| 24 | RA | 996 | A |
| 24 | RA | 1003 | G |
| 24 | RA | 1009 | A |
| 24 | RA | 1012 | U |
| 24 | RA | 1013 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 24 | RA | 1022 | G |
| 24 | RA | 1023 | U |
| 24 | RA | 1025 | G |
| 24 | RA | 1026 | U |
| 24 | RA | 1027 | A |
| 24 | RA | 1033 | U |
| 24 | RA | 1042 | G |
| 24 | RA | 1044 | G |
| 24 | RA | 1045 | A |
| 24 | RA | 1046 | A |
| 24 | RA | 1050 | A |
| 24 | RA | 1053 | C |
| 24 | RA | 1054 | A |
| 24 | RA | 1055 | G |
| 24 | RA | 1057 | A |
| 24 | RA | 1060 | U |
| 24 | RA | 1061 | U |
| 24 | RA | 1065 | U |
| 24 | RA | 1066 | U |
| 24 | RA | 1071 | G |
| 24 | RA | 1073 | A |
| 24 | RA | 1074 | G |
| 24 | RA | 1077 | A |
| 24 | RA | 1078 | U |
| 24 | RA | 1082 | U |
| 24 | RA | 1083 | U |
| 24 | RA | 1084 | A |
| 24 | RA | 1085 | A |
| 24 | RA | 1086 | A |
| 24 | RA | 1087 | G |
| 24 | RA | 1088 | A |
| 24 | RA | 1091 | G |
| 24 | RA | 1093 | G |
| 24 | RA | 1096 | A |
| 24 | RA | 1110 | G |
| 24 | RA | 1111 | A |
| 24 | RA | 1112 | G |
| 24 | RA | 1122 | G |
| 24 | RA | 1130 | U |
| 24 | RA | 1131 | G |
| 24 | RA | 1135 | C |
| 24 | RA | 1136 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 24 | RA | 1140 | C |
| 24 | RA | 1142(A) | A |
| 24 | RA | 1152 | C |
| 24 | RA | 1173 | G |
| 24 | RA | 1174 | A |
| 24 | RA | 1175 | U |
| 24 | RA | 1176 | G |
| 24 | RA | 1178 | C |
| 24 | RA | 1181 | C |
| 24 | RA | 1195 | G |
| 24 | RA | 1204 | A |
| 24 | RA | 1205 | U |
| 24 | RA | 1206 | G |
| 24 | RA | 1210 | A |
| 24 | RA | 1211 | U |
| 24 | RA | 1220 | A |
| 24 | RA | 1236 | G |
| 24 | RA | 1238 | G |
| 24 | RA | 1253 | A |
| 24 | RA | 1256 | G |
| 24 | RA | 1265 | A |
| 24 | RA | 1272 | A |
| 24 | RA | 1273 | U |
| 24 | RA | 1286 | A |
| 24 | RA | 1300 | U |
| 24 | RA | 1301 | A |
| 24 | RA | 1312 | U |
| 24 | RA | 1313 | U |
| 24 | RA | 1314 | C |
| 24 | RA | 1321 | A |
| 24 | RA | 1329 | U |
| 24 | RA | 1341 | U |
| 24 | RA | 1349 | A |
| 24 | RA | 1365 | A |
| 24 | RA | 1370 | C |
| 24 | RA | 1378 | A |
| 24 | RA | 1379 | A |
| 24 | RA | 1380 | G |
| 24 | RA | 1384 | A |
| 24 | RA | 1385 | G |
| 24 | RA | 1390 | U |
| 24 | RA | 1395 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 24 | RA | 1407 | C |
| 24 | RA | 1408 | C |
| 24 | RA | 1411 | C |
| 24 | RA | 1416 | G |
| 24 | RA | 1419 | A |
| 24 | RA | 1420 | U |
| 24 | RA | 1421 | G |
| 24 | RA | 1428 | C |
| 24 | RA | 1444(A) | A |
| 24 | RA | 1445 | C |
| 24 | RA | 1449 | A |
| 24 | RA | 1449(A) | G |
| 24 | RA | 1460 | A |
| 24 | RA | 1461 | G |
| 24 | RA | 1471 | A |
| 24 | RA | 1472 | A |
| 24 | RA | 1473 | G |
| 24 | RA | 1474 | C |
| 24 | RA | 1475 | G |
| 24 | RA | 1480 | G |
| 24 | RA | 1482 | U |
| 24 | RA | 1483 | G |
| 24 | RA | 1487 | G |
| 24 | RA | 1490 | A |
| 24 | RA | 1493 | C |
| 24 | RA | 1494 | A |
| 24 | RA | 1497 | U |
| 24 | RA | 1502 | C |
| 24 | RA | 1504 | C |
| 24 | RA | 1505 | C |
| 24 | RA | 1506 | C |
| 24 | RA | 1507 | A |
| 24 | RA | 1508 | A |
| 24 | RA | 1510 | A |
| 24 | RA | 1513 | C |
| 24 | RA | 1514 | U |
| 24 | RA | 1519 | G |
| 24 | RA | 1520 | U |
| 24 | RA | 1522 | G |
| 24 | RA | 1528 | A |
| 24 | RA | 1535 | U |
| 24 | RA | 1536 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 24 | RA | 1537 | C |
| 24 | RA | 1538 | G |
| 24 | RA | 1543 | A |
| 24 | RA | 1545 | A |
| 24 | RA | 1547 | C |
| 24 | RA | 1558 | A |
| 24 | RA | 1559 | G |
| 24 | RA | 1566 | A |
| 24 | RA | 1569 | A |
| 24 | RA | 1578 | U |
| 24 | RA | 1580 | A |
| 24 | RA | 1581 | G |
| 24 | RA | 1583 | A |
| 24 | RA | 1586 | A |
| 24 | RA | 1598 | C |
| 24 | RA | 1608 | A |
| 24 | RA | 1609 | A |
| 24 | RA | 1616 | A |
| 24 | RA | 1617 | C |
| 24 | RA | 1640 | C |
| 24 | RA | 1646 | C |
| 24 | RA | 1648 | C |
| 24 | RA | 1654 | A |
| 24 | RA | 1665 | A |
| 24 | RA | 1667 | G |
| 24 | RA | 1668 | A |
| 24 | RA | 1674 | G |
| 24 | RA | 1675 | C |
| 24 | RA | 1678 | G |
| 24 | RA | 1725 | G |
| 24 | RA | 1728 | G |
| 24 | RA | 1729 | A |
| 24 | RA | 1733 | G |
| 24 | RA | 1743 | G |
| 24 | RA | 1750 | G |
| 24 | RA | 1756 | G |
| 24 | RA | 1762 | A |
| 24 | RA | 1763 | G |
| 24 | RA | 1764 | G |
| 24 | RA | 1773 | A |
| 24 | RA | 1774 | C |
| 24 | RA | 1780 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 24 | RA | 1781 | C |
| 24 | RA | 1784 | A |
| 24 | RA | 1791 | A |
| 24 | RA | 1799 | G |
| 24 | RA | 1800 | C |
| 24 | RA | 1802 | A |
| 24 | RA | 1816 | G |
| 24 | RA | 1820 | U |
| 24 | RA | 1835 | G |
| 24 | RA | 1847 | A |
| 24 | RA | 1848 | A |
| 24 | RA | 1858 | G |
| 24 | RA | 1869 | G |
| 24 | RA | 1870 | C |
| 24 | RA | 1871 | A |
| 24 | RA | 1872 | A |
| 24 | RA | 1878 | G |
| 24 | RA | 1882 | C |
| 24 | RA | 1884 | A |
| 24 | RA | 1888 | G |
| 24 | RA | 1889 | A |
| 24 | RA | 1906 | G |
| 24 | RA | 1913 | A |
| 24 | RA | 1914 | C |
| 24 | RA | 1929 | G |
| 24 | RA | 1930 | G |
| 24 | RA | 1938 | A |
| 24 | RA | 1939 | U |
| 24 | RA | 1955 | U |
| 24 | RA | 1963 | U |
| 24 | RA | 1967 | C |
| 24 | RA | 1968 | G |
| 24 | RA | 1969 | A |
| 24 | RA | 1970 | A |
| 24 | RA | 1971 | A |
| 24 | RA | 1972 | A |
| 24 | RA | 1981 | A |
| 24 | RA | 1982 | C |
| 24 | RA | 1992 | G |
| 24 | RA | 1993 | U |
| 24 | RA | 1996 | C |
| 24 | RA | 2004 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 24 | RA | 2023 | G |
| 24 | RA | 2031 | A |
| 24 | RA | 2032 | G |
| 24 | RA | 2033 | A |
| 24 | RA | 2043 | C |
| 24 | RA | 2052 | G |
| 24 | RA | 2055 | C |
| 24 | RA | 2056 | G |
| 24 | RA | 2059 | A |
| 24 | RA | 2060 | A |
| 24 | RA | 2061 | G |
| 24 | RA | 2062 | A |
| 24 | RA | 2063 | C |
| 24 | RA | 2069 | G |
| 24 | RA | 2093 | G |
| 24 | RA | 2099 | U |
| 24 | RA | 2101 | G |
| 24 | RA | 2107 | C |
| 24 | RA | 2111 | C |
| 24 | RA | 2113 | U |
| 24 | RA | 2114 | A |
| 24 | RA | 2115 | G |
| 24 | RA | 2116 | G |
| 24 | RA | 2117 | A |
| 24 | RA | 2118 | U |
| 24 | RA | 2126 | A |
| 24 | RA | 2127 | G |
| 24 | RA | 2128 | C |
| 24 | RA | 2131 | G |
| 24 | RA | 2132 | U |
| 24 | RA | 2133 | G |
| 24 | RA | 2135 | A |
| 24 | RA | 2136 | C |
| 24 | RA | 2147 | G |
| 24 | RA | 2148 | G |
| 24 | RA | 2161 | C |
| 24 | RA | 2166 | G |
| 24 | RA | 2168 | G |
| 24 | RA | 2170 | A |
| 24 | RA | 2173 | A |
| 24 | RA | 2189 | U |
| 24 | RA | 2190 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 24 | RA | 2192 | G |
| 24 | RA | 2198 | A |
| 24 | RA | 2199 | A |
| 24 | RA | 2210 | G |
| 24 | RA | 2211 | G |
| 24 | RA | 2212 | A |
| 24 | RA | 2215 | G |
| 24 | RA | 2225 | A |
| 24 | RA | 2238 | G |
| 24 | RA | 2239 | G |
| 24 | RA | 2243 | U |
| 24 | RA | 2275 | C |
| 24 | RA | 2278 | A |
| 24 | RA | 2280 | G |
| 24 | RA | 2283 | C |
| 24 | RA | 2287 | A |
| 24 | RA | 2288 | A |
| 24 | RA | 2307 | G |
| 24 | RA | 2308 | G |
| 24 | RA | 2309 | A |
| 24 | RA | 2311 | A |
| 24 | RA | 2319 | G |
| 24 | RA | 2320 | A |
| 24 | RA | 2325 | G |
| 24 | RA | 2334 | G |
| 24 | RA | 2336 | A |
| 24 | RA | 2342 | C |
| 24 | RA | 2345 | G |
| 24 | RA | 2346 | A |
| 24 | RA | 2347 | C |
| 24 | RA | 2350 | C |
| 24 | RA | 2354 | G |
| 24 | RA | 2383 | G |
| 24 | RA | 2385 | C |
| 24 | RA | 2392 | A |
| 24 | RA | 2396 | G |
| 24 | RA | 2402 | C |
| 24 | RA | 2403 | C |
| 24 | RA | 2406 | U |
| 24 | RA | 2425 | A |
| 24 | RA | 2427 | C |
| 24 | RA | 2428 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 24 | RA | 2429 | G |
| 24 | RA | 2430 | A |
| 24 | RA | 2435 | A |
| 24 | RA | 2439 | A |
| 24 | RA | 2440 | C |
| 24 | RA | 2441 | C |
| 24 | RA | 2447 | G |
| 24 | RA | 2448 | A |
| 24 | RA | 2469 | A |
| 24 | RA | 2470 | G |
| 24 | RA | 2474 | C |
| 24 | RA | 2475 | C |
| 24 | RA | 2478 | A |
| 24 | RA | 2480 | C |
| 24 | RA | 2482 | G |
| 24 | RA | 2494 | G |
| 24 | RA | 2498 | C |
| 24 | RA | 2502 | G |
| 24 | RA | 2505 | G |
| 24 | RA | 2518 | A |
| 24 | RA | 2519 | U |
| 24 | RA | 2529 | G |
| 24 | RA | 2542 | A |
| 24 | RA | 2543 | G |
| 24 | RA | 2554 | U |
| 24 | RA | 2566 | A |
| 24 | RA | 2567 | G |
| 24 | RA | 2569 | G |
| 24 | RA | 2572 | A |
| 24 | RA | 2578 | G |
| 24 | RA | 2582 | G |
| 24 | RA | 2585 | U |
| 24 | RA | 2602 | A |
| 24 | RA | 2609 | U |
| 24 | RA | 2611 | U |
| 24 | RA | 2612 | C |
| 24 | RA | 2623 | G |
| 24 | RA | 2629 | A |
| 24 | RA | 2636 | U |
| 24 | RA | 2641 | G |
| 24 | RA | 2646 | C |
| 24 | RA | 2655 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 24 | RA | 2665 | A |
| 24 | RA | 2673 | G |
| 24 | RA | 2682 | U |
| 24 | RA | 2689 | U |
| 24 | RA | 2690 | C |
| 24 | RA | 2702 | U |
| 24 | RA | 2703 | C |
| 24 | RA | 2712(A) | A |
| 24 | RA | 2713 | A |
| 24 | RA | 2714 | G |
| 24 | RA | 2726 | U |
| 24 | RA | 2733 | A |
| 24 | RA | 2739 | U |
| 24 | RA | 2744 | G |
| 24 | RA | 2748 | A |
| 24 | RA | 2751 | G |
| 24 | RA | 2752 | C |
| 24 | RA | 2757 | A |
| 24 | RA | 2761 | G |
| 24 | RA | 2764 | A |
| 24 | RA | 2765 | A |
| 24 | RA | 2766 | G |
| 24 | RA | 2778 | A |
| 24 | RA | 2779 | U |
| 24 | RA | 2789 | C |
| 24 | RA | 2790 | A |
| 24 | RA | 2791 | C |
| 24 | RA | 2797 | U |
| 24 | RA | 2798 | C |
| 24 | RA | 2807 | G |
| 24 | RA | 2818 | G |
| 24 | RA | 2820 | A |
| 24 | RA | 2821 | A |
| 24 | RA | 2833 | G |
| 24 | RA | 2834 | G |
| 24 | RA | 2849 | U |
| 24 | RA | 2867 | G |
| 24 | RA | 2872 | G |
| 24 | RA | 2880 | C |
| 24 | RA | 2891 | G |
| 24 | RA | 2892 | A |
| 24 | RA | 2894 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 24 | RA | 2895 | U |
| 24 | RA | 2897 | U |
| 25 | RB | 8 | U |
| 25 | RB | 9 | G |
| 25 | RB | 13 | A |
| 25 | RB | 15 | A |
| 25 | RB | 19 | G |
| 25 | RB | 21 | G |
| 25 | RB | 24 | G |
| 25 | RB | 25 | A |
| 25 | RB | 41 | U |
| 25 | RB | 42 | C |
| 25 | RB | 44 | G |
| 25 | RB | 45 | A |
| 25 | RB | 52 | A |
| 25 | RB | 56 | G |
| 25 | RB | 67 | G |
| 25 | RB | 73 | A |
| 25 | RB | 108 | C |
| 25 | RB | 109 | G |
| 1 | XA | 6 | G |
| 1 | XA | 32 | A |
| 1 | XA | 35 | G |
| 1 | XA | 39 | G |
| 1 | XA | 47 | C |
| 1 | XA | 48 | C |
| 1 | XA | 50 | A |
| 1 | XA | 51 | A |
| 1 | XA | 61 | G |
| 1 | XA | 65 | U |
| 1 | XA | 66 | G |
| 1 | XA | 78 | G |
| 1 | XA | 79 | G |
| 1 | XA | 89 | U |
| 1 | XA | 92 | G |
| 1 | XA | 95 | G |
| 1 | XA | 101 | A |
| 1 | XA | 115 | G |
| 1 | XA | 116 | A |
| 1 | XA | 121 | C |
| 1 | XA | 130 | A |
| 1 | XA | 144 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | XA | 147 | G |
| 1 | XA | 160 | A |
| 1 | XA | 161 | A |
| 1 | XA | 163 | C |
| 1 | XA | 169 | C |
| 1 | XA | 172 | A |
| 1 | XA | 173 | U |
| 1 | XA | 174 | C |
| 1 | XA | 190 | G |
| 1 | XA | 195 | A |
| 1 | XA | 197 | A |
| 1 | XA | 201 | C |
| 1 | XA | 209 | U |
| 1 | XA | 210 | U |
| 1 | XA | 244 | U |
| 1 | XA | 245 | C |
| 1 | XA | 247 | G |
| 1 | XA | 251 | G |
| 1 | XA | 267 | C |
| 1 | XA | 270 | A |
| 1 | XA | 281 | G |
| 1 | XA | 289 | G |
| 1 | XA | 306 | G |
| 1 | XA | 314 | C |
| 1 | XA | 321 | A |
| 1 | XA | 328 | C |
| 1 | XA | 329 | A |
| 1 | XA | 332 | G |
| 1 | XA | 346 | G |
| 1 | XA | 347 | G |
| 1 | XA | 351 | G |
| 1 | XA | 352 | C |
| 1 | XA | 353 | A |
| 1 | XA | 354 | G |
| 1 | XA | 356 | A |
| 1 | XA | 367 | U |
| 1 | XA | 372 | C |
| 1 | XA | 373 | A |
| 1 | XA | 389 | A |
| 1 | XA | 397 | A |
| 1 | XA | 398 | C |
| 1 | XA | 406 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | XA | 411 | A |
| 1 | XA | 412 | A |
| 1 | XA | 413 | G |
| 1 | XA | 422 | C |
| 1 | XA | 423 | G |
| 1 | XA | 428 | G |
| 1 | XA | 429 | U |
| 1 | XA | 435 | C |
| 1 | XA | 452 | A |
| 1 | XA | 465 | A |
| 1 | XA | 466 | C |
| 1 | XA | 467 | G |
| 1 | XA | 482 | A |
| 1 | XA | 485 | G |
| 1 | XA | 486 | U |
| 1 | XA | 496 | A |
| 1 | XA | 497 | U |
| 1 | XA | 509 | A |
| 1 | XA | 510 | A |
| 1 | XA | 511 | C |
| 1 | XA | 518 | C |
| 1 | XA | 521 | G |
| 1 | XA | 527 | G |
| 1 | XA | 531 | U |
| 1 | XA | 532 | A |
| 1 | XA | 533 | A |
| 1 | XA | 547 | A |
| 1 | XA | 548 | G |
| 1 | XA | 559 | A |
| 1 | XA | 561 | U |
| 1 | XA | 562 | C |
| 1 | XA | 564 | C |
| 1 | XA | 568 | G |
| 1 | XA | 572 | A |
| 1 | XA | 573 | A |
| 1 | XA | 574 | A |
| 1 | XA | 576 | G |
| 1 | XA | 577 | G |
| 1 | XA | 618 | C |
| 1 | XA | 630 | G |
| 1 | XA | 631 | G |
| 1 | XA | 632 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | XA | 653 | A |
| 1 | XA | 665 | A |
| 1 | XA | 688 | G |
| 1 | XA | 702 | A |
| 1 | XA | 703 | G |
| 1 | XA | 704 | A |
| 1 | XA | 721 | G |
| 1 | XA | 723 | U |
| 1 | XA | 731 | G |
| 1 | XA | 749 | C |
| 1 | XA | 754 | C |
| 1 | XA | 755 | G |
| 1 | XA | 777 | A |
| 1 | XA | 792 | A |
| 1 | XA | 793 | U |
| 1 | XA | 794 | A |
| 1 | XA | 813 | U |
| 1 | XA | 816 | A |
| 1 | XA | 817 | C |
| 1 | XA | 818 | G |
| 1 | XA | 821 | G |
| 1 | XA | 828 | A |
| 1 | XA | 841 | U |
| 1 | XA | 842 | C |
| 1 | XA | 843 | U |
| 1 | XA | 848 | C |
| 1 | XA | 859 | A |
| 1 | XA | 871 | U |
| 1 | XA | 872 | A |
| 1 | XA | 902 | G |
| 1 | XA | 914 | A |
| 1 | XA | 926 | G |
| 1 | XA | 927 | G |
| 1 | XA | 934 | C |
| 1 | XA | 958 | A |
| 1 | XA | 960 | U |
| 1 | XA | 968 | A |
| 1 | XA | 969 | A |
| 1 | XA | 972 | C |
| 1 | XA | 974 | A |
| 1 | XA | 975 | A |
| 1 | XA | 976 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | XA | 977 | A |
| 1 | XA | 991 | U |
| 1 | XA | 992 | U |
| 1 | XA | 993 | G |
| 1 | XA | 1004 | A |
| 1 | XA | 1006 | C |
| 1 | XA | 1009 | G |
| 1 | XA | 1024 | G |
| 1 | XA | 1025 | U |
| 1 | XA | 1028 | C |
| 1 | XA | 1029 | G |
| 1 | XA | 1031 | G |
| 1 | XA | 1032 | A |
| 1 | XA | 1032(A) | G |
| 1 | XA | 1039 | C |
| 1 | XA | 1040 | U |
| 1 | XA | 1042 | G |
| 1 | XA | 1053 | G |
| 1 | XA | 1054 | C |
| 1 | XA | 1066 | C |
| 1 | XA | 1081 | G |
| 1 | XA | 1094 | G |
| 1 | XA | 1095 | U |
| 1 | XA | 1101 | A |
| 1 | XA | 1104 | G |
| 1 | XA | 1108 | G |
| 1 | XA | 1124 | G |
| 1 | XA | 1125 | U |
| 1 | XA | 1126 | U |
| 1 | XA | 1127 | G |
| 1 | XA | 1129 | C |
| 1 | XA | 1130 | A |
| 1 | XA | 1131 | G |
| 1 | XA | 1136 | U |
| 1 | XA | 1137 | C |
| 1 | XA | 1138 | G |
| 1 | XA | 1139 | G |
| 1 | XA | 1146 | A |
| 1 | XA | 1157 | A |
| 1 | XA | 1158 | C |
| 1 | XA | 1159 | U |
| 1 | XA | 1160 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | XA | 1162 | C |
| 1 | XA | 1176 | A |
| 1 | XA | 1177 | G |
| 1 | XA | 1181 | G |
| 1 | XA | 1183 | A |
| 1 | XA | 1184 | G |
| 1 | XA | 1187 | G |
| 1 | XA | 1196 | U |
| 1 | XA | 1199 | U |
| 1 | XA | 1200 | C |
| 1 | XA | 1212 | U |
| 1 | XA | 1224 | G |
| 1 | XA | 1238 | A |
| 1 | XA | 1240 | U |
| 1 | XA | 1241 | G |
| 1 | XA | 1256 | A |
| 1 | XA | 1257 | U |
| 1 | XA | 1258 | G |
| 1 | XA | 1260 | C |
| 1 | XA | 1263 | C |
| 1 | XA | 1270 | C |
| 1 | XA | 1273 | G |
| 1 | XA | 1280 | A |
| 1 | XA | 1281 | U |
| 1 | XA | 1286 | A |
| 1 | XA | 1287 | A |
| 1 | XA | 1298 | C |
| 1 | XA | 1300 | G |
| 1 | XA | 1302 | U |
| 1 | XA | 1303 | C |
| 1 | XA | 1305 | G |
| 1 | XA | 1310 | G |
| 1 | XA | 1311 | G |
| 1 | XA | 1319 | A |
| 1 | XA | 1320 | C |
| 1 | XA | 1321 | C |
| 1 | XA | 1322 | C |
| 1 | XA | 1323 | G |
| 1 | XA | 1331 | G |
| 1 | XA | 1336 | C |
| 1 | XA | 1337 | G |
| 1 | XA | 1346 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | XA | 1347 | G |
| 1 | XA | 1362(A) | C |
| 1 | XA | 1364 | U |
| 1 | XA | 1381 | U |
| 1 | XA | 1419 | G |
| 1 | XA | 1442 | G |
| 1 | XA | 1446 | A |
| 1 | XA | 1447 | G |
| 1 | XA | 1452 | C |
| 1 | XA | 1453 | G |
| 1 | XA | 1454 | G |
| 1 | XA | 1492 | A |
| 1 | XA | 1493 | A |
| 1 | XA | 1499 | A |
| 1 | XA | 1502 | A |
| 1 | XA | 1504 | G |
| 1 | XA | 1505 | G |
| 1 | XA | 1506 | U |
| 1 | XA | 1517 | G |
| 1 | XA | 1520 | G |
| 1 | XA | 1529 | G |
| 1 | XA | 1530 | G |
| 23 | XX | 7 | G |
| 23 | XX | 11 | U |
| 23 | XX | 12 | A |
| 23 | XX | 13 | A |
| 23 | XX | 14 | A |
| 24 | YA | 9 | U |
| 24 | YA | 15 | G |
| 24 | YA | 34 | C |
| 24 | YA | 35 | G |
| 24 | YA | 46 | C |
| 24 | YA | 55 | G |
| 24 | YA | 61 | G |
| 24 | YA | 63 | U |
| 24 | YA | 72 | U |
| 24 | YA | 74 | A |
| 24 | YA | 75 | G |
| 24 | YA | 101 | G |
| 24 | YA | 102 | G |
| 24 | YA | 103 | A |
| 24 | YA | 118 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 24 | YA | 120 | U |
| 24 | YA | 125 | G |
| 24 | YA | 140 | A |
| 24 | YA | 161 | U |
| 24 | YA | 162 | U |
| 24 | YA | 181 | A |
| 24 | YA | 196 | A |
| 24 | YA | 199 | A |
| 24 | YA | 214 | G |
| 24 | YA | 216 | A |
| 24 | YA | 221 | A |
| 24 | YA | 222 | A |
| 24 | YA | 223 | A |
| 24 | YA | 226 | G |
| 24 | YA | 228 | A |
| 24 | YA | 229 | A |
| 24 | YA | 230 | U |
| 24 | YA | 232 | G |
| 24 | YA | 241 | A |
| 24 | YA | 242 | G |
| 24 | YA | 243 | U |
| 24 | YA | 248 | G |
| 24 | YA | 249 | C |
| 24 | YA | 252 | G |
| 24 | YA | 265 | A |
| 24 | YA | 266 | G |
| 24 | YA | 270(L) | U |
| 24 | YA | 270(M) | U |
| 24 | YA | 270(N) | G |
| 24 | YA | 270(P) | C |
| 24 | YA | 271(C) | U |
| 24 | YA | 271(D) | G |
| 24 | YA | 274 | G |
| 24 | YA | 275 | G |
| 24 | YA | 276 | A |
| 24 | YA | 278 | A |
| 24 | YA | 279 | C |
| 24 | YA | 299 | A |
| 24 | YA | 300 | A |
| 24 | YA | 311 | A |
| 24 | YA | 323 | G |
| 24 | YA | 324 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 24 | YA | 329 | G |
| 24 | YA | 330 | A |
| 24 | YA | 332 | A |
| 24 | YA | 352 | G |
| 24 | YA | 363 | G |
| 24 | YA | 363(E) | U |
| 24 | YA | 364 | C |
| 24 | YA | 371 | A |
| 24 | YA | 372 | G |
| 24 | YA | 386 | G |
| 24 | YA | 387 | U |
| 24 | YA | 395 | U |
| 24 | YA | 405 | U |
| 24 | YA | 406 | G |
| 24 | YA | 411 | G |
| 24 | YA | 412 | A |
| 24 | YA | 428 | A |
| 24 | YA | 443 | A |
| 24 | YA | 444 | C |
| 24 | YA | 448 | U |
| 24 | YA | 451 | C |
| 24 | YA | 457 | A |
| 24 | YA | 458 | G |
| 24 | YA | 467 | G |
| 24 | YA | 470 | A |
| 24 | YA | 481 | G |
| 24 | YA | 504 | U |
| 24 | YA | 505 | A |
| 24 | YA | 509 | C |
| 24 | YA | 511 | U |
| 24 | YA | 518 | G |
| 24 | YA | 527 | C |
| 24 | YA | 529 | A |
| 24 | YA | 530 | G |
| 24 | YA | 531 | C |
| 24 | YA | 532 | A |
| 24 | YA | 533 | G |
| 24 | YA | 537 | C |
| 24 | YA | 539 | G |
| 24 | YA | 540 | G |
| 24 | YA | 546 | C |
| 24 | YA | 547 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 24 | YA | 563 | G |
| 24 | YA | 566 | U |
| 24 | YA | 568 | U |
| 24 | YA | 571 | A |
| 24 | YA | 573 | G |
| 24 | YA | 575 | A |
| 24 | YA | 600 | G |
| 24 | YA | 603 | A |
| 24 | YA | 607 | U |
| 24 | YA | 614 | U |
| 24 | YA | 617 | G |
| 24 | YA | 621 | A |
| 24 | YA | 627 | A |
| 24 | YA | 637 | A |
| 24 | YA | 638 | G |
| 24 | YA | 645 | C |
| 24 | YA | 646 | A |
| 24 | YA | 647 | G |
| 24 | YA | 651 | G |
| 24 | YA | 654 | A |
| 24 | YA | 654(A) | G |
| 24 | YA | 668 | G |
| 24 | YA | 669 | G |
| 24 | YA | 686 | G |
| 24 | YA | 717 | G |
| 24 | YA | 722 | A |
| 24 | YA | 726 | G |
| 24 | YA | 730 | C |
| 24 | YA | 753 | C |
| 24 | YA | 764 | A |
| 24 | YA | 765 | G |
| 24 | YA | 782 | A |
| 24 | YA | 784 | A |
| 24 | YA | 785 | G |
| 24 | YA | 789 | A |
| 24 | YA | 790 | C |
| 24 | YA | 791 | C |
| 24 | YA | 792 | G |
| 24 | YA | 805 | G |
| 24 | YA | 812 | C |
| 24 | YA | 819 | A |
| 24 | YA | 827 | U |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 24 | YA | 828 | U |
| 24 | YA | 831 | G |
| 24 | YA | 847 | U |
| 24 | YA | 856 | C |
| 24 | YA | 857 | C |
| 24 | YA | 859 | G |
| 24 | YA | 860 | U |
| 24 | YA | 866 | A |
| 24 | YA | 880 | G |
| 24 | YA | 881 | G |
| 24 | YA | 882 | G |
| 24 | YA | 884 | C |
| 24 | YA | 885 | C |
| 24 | YA | 886 | C |
| 24 | YA | 888 | C |
| 24 | YA | 889 | C |
| 24 | YA | 896 | A |
| 24 | YA | 897 | C |
| 24 | YA | 900 | A |
| 24 | YA | 907 | U |
| 24 | YA | 910 | A |
| 24 | YA | 915 | C |
| 24 | YA | 917 | A |
| 24 | YA | 941 | A |
| 24 | YA | 945 | A |
| 24 | YA | 946 | G |
| 24 | YA | 953 | A |
| 24 | YA | 957 | A |
| 24 | YA | 959 | A |
| 24 | YA | 961 | C |
| 24 | YA | 973 | A |
| 24 | YA | 974 | G |
| 24 | YA | 974(A) | C |
| 24 | YA | 975 | G |
| 24 | YA | 980 | A |
| 24 | YA | 983 | A |
| 24 | YA | 996 | A |
| 24 | YA | 1005 | C |
| 24 | YA | 1009 | A |
| 24 | YA | 1010 | A |
| 24 | YA | 1011 | G |
| 24 | YA | 1012 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 24 | YA | 1013 | C |
| 24 | YA | 1022 | G |
| 24 | YA | 1023 | U |
| 24 | YA | 1026 | U |
| 24 | YA | 1027 | A |
| 24 | YA | 1033 | U |
| 24 | YA | 1046 | A |
| 24 | YA | 1047 | G |
| 24 | YA | 1050 | A |
| 24 | YA | 1054 | A |
| 24 | YA | 1059 | G |
| 24 | YA | 1060 | U |
| 24 | YA | 1061 | U |
| 24 | YA | 1062 | G |
| 24 | YA | 1065 | U |
| 24 | YA | 1067 | A |
| 24 | YA | 1068 | G |
| 24 | YA | 1070 | A |
| 24 | YA | 1071 | G |
| 24 | YA | 1073 | A |
| 24 | YA | 1077 | A |
| 24 | YA | 1078 | U |
| 24 | YA | 1082 | U |
| 24 | YA | 1083 | U |
| 24 | YA | 1084 | A |
| 24 | YA | 1085 | A |
| 24 | YA | 1086 | A |
| 24 | YA | 1088 | A |
| 24 | YA | 1089 | G |
| 24 | YA | 1093 | G |
| 24 | YA | 1096 | A |
| 24 | YA | 1097 | U |
| 24 | YA | 1103 | A |
| 24 | YA | 1104 | C |
| 24 | YA | 1110 | G |
| 24 | YA | 1111 | A |
| 24 | YA | 1122 | G |
| 24 | YA | 1126 | A |
| 24 | YA | 1130 | U |
| 24 | YA | 1135 | C |
| 24 | YA | 1136 | G |
| 24 | YA | 1139 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 24 | YA | 1142 | U |
| 24 | YA | 1142(A) | A |
| 24 | YA | 1151 | G |
| 24 | YA | 1169 | G |
| 24 | YA | 1173 | G |
| 24 | YA | 1174 | A |
| 24 | YA | 1175 | U |
| 24 | YA | 1176 | G |
| 24 | YA | 1179 | C |
| 24 | YA | 1180 | C |
| 24 | YA | 1204 | A |
| 24 | YA | 1205 | U |
| 24 | YA | 1211 | U |
| 24 | YA | 1220 | A |
| 24 | YA | 1221 | C |
| 24 | YA | 1236 | G |
| 24 | YA | 1238 | G |
| 24 | YA | 1244 | G |
| 24 | YA | 1248 | G |
| 24 | YA | 1250 | G |
| 24 | YA | 1253 | A |
| 24 | YA | 1256 | G |
| 24 | YA | 1265 | A |
| 24 | YA | 1271 | G |
| 24 | YA | 1272 | A |
| 24 | YA | 1273 | U |
| 24 | YA | 1300 | U |
| 24 | YA | 1301 | A |
| 24 | YA | 1325 | G |
| 24 | YA | 1329 | U |
| 24 | YA | 1349 | A |
| 24 | YA | 1352 | U |
| 24 | YA | 1355 | G |
| 24 | YA | 1365 | A |
| 24 | YA | 1368 | G |
| 24 | YA | 1370 | C |
| 24 | YA | 1378 | A |
| 24 | YA | 1379 | A |
| 24 | YA | 1384 | A |
| 24 | YA | 1385 | G |
| 24 | YA | 1392 | A |
| 24 | YA | 1395 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 24 | YA | 1407 | C |
| 24 | YA | 1411 | C |
| 24 | YA | 1412 | A |
| 24 | YA | 1416 | G |
| 24 | YA | 1419 | A |
| 24 | YA | 1420 | U |
| 24 | YA | 1421 | G |
| 24 | YA | 1428 | C |
| 24 | YA | 1444(A) | A |
| 24 | YA | 1445 | C |
| 24 | YA | 1449 | A |
| 24 | YA | 1449(A) | G |
| 24 | YA | 1455 | G |
| 24 | YA | 1459 | G |
| 24 | YA | 1460 | A |
| 24 | YA | 1461 | G |
| 24 | YA | 1467 | C |
| 24 | YA | 1471 | A |
| 24 | YA | 1478 | G |
| 24 | YA | 1482 | U |
| 24 | YA | 1483 | G |
| 24 | YA | 1487 | G |
| 24 | YA | 1490 | A |
| 24 | YA | 1493 | C |
| 24 | YA | 1494 | A |
| 24 | YA | 1496 | A |
| 24 | YA | 1497 | U |
| 24 | YA | 1507 | A |
| 24 | YA | 1508 | A |
| 24 | YA | 1509 | C |
| 24 | YA | 1510 | A |
| 24 | YA | 1511 | A |
| 24 | YA | 1515 | C |
| 24 | YA | 1517 | G |
| 24 | YA | 1520 | U |
| 24 | YA | 1522 | G |
| 24 | YA | 1534 | G |
| 24 | YA | 1535 | U |
| 24 | YA | 1536 | A |
| 24 | YA | 1537 | C |
| 24 | YA | 1540 | G |
| 24 | YA | 1543 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 24 | YA | 1544 | C |
| 24 | YA | 1545 | A |
| 24 | YA | 1546 | C |
| 24 | YA | 1558 | A |
| 24 | YA | 1559 | G |
| 24 | YA | 1566 | A |
| 24 | YA | 1569 | A |
| 24 | YA | 1578 | U |
| 24 | YA | 1580 | A |
| 24 | YA | 1581 | G |
| 24 | YA | 1585 | C |
| 24 | YA | 1586 | A |
| 24 | YA | 1591 | G |
| 24 | YA | 1598 | C |
| 24 | YA | 1608 | A |
| 24 | YA | 1609 | A |
| 24 | YA | 1610 | A |
| 24 | YA | 1616 | A |
| 24 | YA | 1617 | C |
| 24 | YA | 1618 | A |
| 24 | YA | 1640 | C |
| 24 | YA | 1646 | C |
| 24 | YA | 1647 | G |
| 24 | YA | 1648 | C |
| 24 | YA | 1654 | A |
| 24 | YA | 1669 | A |
| 24 | YA | 1670 | C |
| 24 | YA | 1674 | G |
| 24 | YA | 1675 | C |
| 24 | YA | 1693 | U |
| 24 | YA | 1695 | G |
| 24 | YA | 1725 | G |
| 24 | YA | 1728 | G |
| 24 | YA | 1729 | A |
| 24 | YA | 1730 | U |
| 24 | YA | 1731 | G |
| 24 | YA | 1732 | A |
| 24 | YA | 1743 | G |
| 24 | YA | 1750 | G |
| 24 | YA | 1753 | G |
| 24 | YA | 1754 | C |
| 24 | YA | 1756 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 24 | YA | 1762 | A |
| 24 | YA | 1763 | G |
| 24 | YA | 1764 | G |
| 24 | YA | 1773 | A |
| 24 | YA | 1779 | U |
| 24 | YA | 1780 | A |
| 24 | YA | 1781 | C |
| 24 | YA | 1784 | A |
| 24 | YA | 1787 | A |
| 24 | YA | 1791 | A |
| 24 | YA | 1799 | G |
| 24 | YA | 1800 | C |
| 24 | YA | 1801 | G |
| 24 | YA | 1815 | A |
| 24 | YA | 1816 | G |
| 24 | YA | 1829 | A |
| 24 | YA | 1835 | G |
| 24 | YA | 1847 | A |
| 24 | YA | 1858 | G |
| 24 | YA | 1869 | G |
| 24 | YA | 1870 | C |
| 24 | YA | 1871 | A |
| 24 | YA | 1872 | A |
| 24 | YA | 1878 | G |
| 24 | YA | 1882 | C |
| 24 | YA | 1889 | A |
| 24 | YA | 1899 | G |
| 24 | YA | 1903 | G |
| 24 | YA | 1906 | G |
| 24 | YA | 1914 | C |
| 24 | YA | 1919 | A |
| 24 | YA | 1929 | G |
| 24 | YA | 1930 | G |
| 24 | YA | 1931 | U |
| 24 | YA | 1936 | A |
| 24 | YA | 1938 | A |
| 24 | YA | 1939 | U |
| 24 | YA | 1940 | U |
| 24 | YA | 1955 | U |
| 24 | YA | 1956 | U |
| 24 | YA | 1960 | A |
| 24 | YA | 1963 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 24 | YA | 1967 | C |
| 24 | YA | 1968 | G |
| 24 | YA | 1969 | A |
| 24 | YA | 1970 | A |
| 24 | YA | 1971 | A |
| 24 | YA | 1972 | A |
| 24 | YA | 1982 | C |
| 24 | YA | 1992 | G |
| 24 | YA | 1993 | U |
| 24 | YA | 2020 | A |
| 24 | YA | 2021 | C |
| 24 | YA | 2023 | G |
| 24 | YA | 2031 | A |
| 24 | YA | 2033 | A |
| 24 | YA | 2043 | C |
| 24 | YA | 2052 | G |
| 24 | YA | 2055 | C |
| 24 | YA | 2056 | G |
| 24 | YA | 2059 | A |
| 24 | YA | 2060 | A |
| 24 | YA | 2061 | G |
| 24 | YA | 2062 | A |
| 24 | YA | 2069 | G |
| 24 | YA | 2093 | G |
| 24 | YA | 2100 | G |
| 24 | YA | 2111 | C |
| 24 | YA | 2112 | G |
| 24 | YA | 2114 | A |
| 24 | YA | 2115 | G |
| 24 | YA | 2116 | G |
| 24 | YA | 2118 | U |
| 24 | YA | 2119 | A |
| 24 | YA | 2120 | G |
| 24 | YA | 2126 | A |
| 24 | YA | 2127 | G |
| 24 | YA | 2131 | G |
| 24 | YA | 2132 | U |
| 24 | YA | 2133 | G |
| 24 | YA | 2136 | C |
| 24 | YA | 2146 | C |
| 24 | YA | 2147 | G |
| 24 | YA | 2148 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 24 | YA | 2156 | G |
| 24 | YA | 2157 | G |
| 24 | YA | 2158 | A |
| 24 | YA | 2166 | G |
| 24 | YA | 2167 | U |
| 24 | YA | 2168 | G |
| 24 | YA | 2169 | A |
| 24 | YA | 2171 | A |
| 24 | YA | 2173 | A |
| 24 | YA | 2176 | A |
| 24 | YA | 2180 | U |
| 24 | YA | 2189 | U |
| 24 | YA | 2190 | G |
| 24 | YA | 2192 | G |
| 24 | YA | 2198 | A |
| 24 | YA | 2210 | G |
| 24 | YA | 2211 | G |
| 24 | YA | 2212 | A |
| 24 | YA | 2213 | U |
| 24 | YA | 2215 | G |
| 24 | YA | 2225 | A |
| 24 | YA | 2238 | G |
| 24 | YA | 2239 | G |
| 24 | YA | 2243 | U |
| 24 | YA | 2266 | A |
| 24 | YA | 2275 | C |
| 24 | YA | 2279 | G |
| 24 | YA | 2280 | G |
| 24 | YA | 2283 | C |
| 24 | YA | 2287 | A |
| 24 | YA | 2288 | A |
| 24 | YA | 2307 | G |
| 24 | YA | 2308 | G |
| 24 | YA | 2309 | A |
| 24 | YA | 2311 | A |
| 24 | YA | 2320 | A |
| 24 | YA | 2325 | G |
| 24 | YA | 2334 | G |
| 24 | YA | 2335 | A |
| 24 | YA | 2343 | C |
| 24 | YA | 2345 | G |
| 24 | YA | 2346 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 24 | YA | 2347 | C |
| 24 | YA | 2350 | C |
| 24 | YA | 2354 | G |
| 24 | YA | 2372 | G |
| 24 | YA | 2383 | G |
| 24 | YA | 2385 | C |
| 24 | YA | 2392 | A |
| 24 | YA | 2396 | G |
| 24 | YA | 2402 | C |
| 24 | YA | 2403 | C |
| 24 | YA | 2406 | U |
| 24 | YA | 2410 | G |
| 24 | YA | 2423 | U |
| 24 | YA | 2425 | A |
| 24 | YA | 2427 | C |
| 24 | YA | 2428 | G |
| 24 | YA | 2429 | G |
| 24 | YA | 2430 | A |
| 24 | YA | 2435 | A |
| 24 | YA | 2439 | A |
| 24 | YA | 2441 | C |
| 24 | YA | 2447 | G |
| 24 | YA | 2448 | A |
| 24 | YA | 2450 | A |
| 24 | YA | 2469 | A |
| 24 | YA | 2475 | C |
| 24 | YA | 2478 | A |
| 24 | YA | 2494 | G |
| 24 | YA | 2498 | C |
| 24 | YA | 2502 | G |
| 24 | YA | 2504 | U |
| 24 | YA | 2505 | G |
| 24 | YA | 2518 | A |
| 24 | YA | 2542 | A |
| 24 | YA | 2543 | G |
| 24 | YA | 2554 | U |
| 24 | YA | 2566 | A |
| 24 | YA | 2567 | G |
| 24 | YA | 2572 | A |
| 24 | YA | 2573 | C |
| 24 | YA | 2582 | G |
| 24 | YA | 2602 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 24 | YA | 2609 | U |
| 24 | YA | 2611 | U |
| 24 | YA | 2612 | C |
| 24 | YA | 2615 | U |
| 24 | YA | 2629 | A |
| 24 | YA | 2654 | A |
| 24 | YA | 2655 | G |
| 24 | YA | 2656 | U |
| 24 | YA | 2665 | A |
| 24 | YA | 2673 | G |
| 24 | YA | 2682 | U |
| 24 | YA | 2689 | U |
| 24 | YA | 2701 | C |
| 24 | YA | 2702 | U |
| 24 | YA | 2707 | G |
| 24 | YA | 2712 | U |
| 24 | YA | 2712(A) | A |
| 24 | YA | 2713 | A |
| 24 | YA | 2714 | G |
| 24 | YA | 2724 | C |
| 24 | YA | 2726 | U |
| 24 | YA | 2733 | A |
| 24 | YA | 2739 | U |
| 24 | YA | 2744 | G |
| 24 | YA | 2748 | A |
| 24 | YA | 2749 | A |
| 24 | YA | 2751 | G |
| 24 | YA | 2757 | A |
| 24 | YA | 2762 | G |
| 24 | YA | 2764 | A |
| 24 | YA | 2765 | A |
| 24 | YA | 2766 | G |
| 24 | YA | 2777 | G |
| 24 | YA | 2778 | A |
| 24 | YA | 2779 | U |
| 24 | YA | 2790 | A |
| 24 | YA | 2791 | C |
| 24 | YA | 2797 | U |
| 24 | YA | 2807 | G |
| 24 | YA | 2808 | U |
| 24 | YA | 2818 | G |
| 24 | YA | 2820 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 24 | YA | 2821 | A |
| 24 | YA | 2833 | G |
| 24 | YA | 2834 | G |
| 24 | YA | 2835 | A |
| 24 | YA | 2836 | U |
| 24 | YA | 2845 | G |
| 24 | YA | 2847 | U |
| 24 | YA | 2867 | G |
| 24 | YA | 2868 | A |
| 24 | YA | 2872 | G |
| 24 | YA | 2879 | C |
| 24 | YA | 2891 | G |
| 24 | YA | 2892 | A |
| 24 | YA | 2893 | G |
| 24 | YA | 2894 | G |
| 25 | YB | 8 | U |
| 25 | YB | 9 | G |
| 25 | YB | 13 | A |
| 25 | YB | 15 | A |
| 25 | YB | 16 | G |
| 25 | YB | 19 | G |
| 25 | YB | 25 | A |
| 25 | YB | 40 | U |
| 25 | YB | 41 | U |
| 25 | YB | 42 | C |
| 25 | YB | 44 | G |
| 25 | YB | 45 | A |
| 25 | YB | 52 | A |
| 25 | YB | 56 | G |
| 25 | YB | 67 | G |
| 25 | YB | 73 | A |
| 25 | YB | 81 | G |
| 25 | YB | 82 | G |
| 25 | YB | 89 | G |
| 25 | YB | 108 | C |
| 25 | YB | 109 | G |
| 22 | XV | 4 | U |
| 22 | XV | 5 | G |
| 22 | XV | 8 | U |
| 22 | XV | 18 | U |
| 22 | XV | 19 | G |
| 22 | XV | 20 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | XV | 22 | A |
| 22 | XV | 48 | U |
| 22 | XV | 49 | C |
| 22 | XV | 55 | U |
| 22 | XV | 58 | G |
| 22 | XV | 64 | U |
| 22 | XV | 65 | C |
| 22 | XV | 66 | U |
| 22 | XV | 68 | U |
| 22 | XV | 76 | C |
| 22 | XV | 77 | A |

All (157) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | QA | 5 | U |
| 1 | QA | 64 | G |
| 1 | QA | 115 | G |
| 1 | QA | 119 | A |
| 1 | QA | 181 | G |
| 1 | QA | 243 | A |
| 1 | QA | 244 | U |
| 1 | QA | 250 | A |
| 1 | QA | 266 | G |
| 1 | QA | 328 | C |
| 1 | QA | 410 | G |
| 1 | QA | 412 | A |
| 1 | QA | 429 | U |
| 1 | QA | 481 | G |
| 1 | QA | 484 | G |
| 1 | QA | 485 | G |
| 1 | QA | 509 | A |
| 1 | QA | 687 | A |
| 1 | QA | 703 | G |
| 1 | QA | 753 | A |
| 1 | QA | 792 | A |
| 1 | QA | 812 | C |
| 1 | QA | 913 | A |
| 1 | QA | 960 | U |
| 1 | QA | 992 | U |
| 1 | QA | 1064 | G |
| 1 | QA | 1065 | U |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | QA | 1200 | C |
| 1 | QA | 1201 | A |
| 1 | QA | 1285 | A |
| 1 | QA | 1297 | C |
| 1 | QA | 1336 | C |
| 1 | QA | 1346 | A |
| 1 | QA | 1347 | G |
| 1 | QA | 1446 | A |
| 1 | QA | 1498 | U |
| 1 | QA | 1528 | U |
| 22 | QV | 54 | G |
| 23 | QX | 15 | A |
| 23 | QX | 21 | G |
| 24 | RA | 74 | A |
| 24 | RA | 99 | U |
| 24 | RA | 221 | A |
| 24 | RA | 222 | A |
| 24 | RA | 229 | A |
| 24 | RA | 271(B) | G |
| 24 | RA | 345 | A |
| 24 | RA | 372 | G |
| 24 | RA | 404 | C |
| 24 | RA | 503 | A |
| 24 | RA | 508 | G |
| 24 | RA | 512 | G |
| 24 | RA | 587 | C |
| 24 | RA | 637 | A |
| 24 | RA | 730 | C |
| 24 | RA | 752 | A |
| 24 | RA | 774 | A |
| 24 | RA | 846 | C |
| 24 | RA | 856 | C |
| 24 | RA | 1022 | G |
| 24 | RA | 1026 | U |
| 24 | RA | 1045 | A |
| 24 | RA | 1085 | A |
| 24 | RA | 1210 | A |
| 24 | RA | 1312 | U |
| 24 | RA | 1427 | A |
| 24 | RA | 1473 | G |
| 24 | RA | 1558 | A |
| 24 | RA | 1653 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 24 | RA | 1819 | A |
| 24 | RA | 1980 | G |
| 24 | RA | 1992 | G |
| 24 | RA | 2060 | A |
| 24 | RA | 2126 | A |
| 24 | RA | 2439 | A |
| 24 | RA | 2566 | A |
| 24 | RA | 2582 | G |
| 24 | RA | 2610 | C |
| 24 | RA | 2689 | U |
| 24 | RA | 2756 | U |
| 24 | RA | 2832 | U |
| 25 | RB | 66 | A |
| 1 | XA | 60 | A |
| 1 | XA | 64 | G |
| 1 | XA | 78 | G |
| 1 | XA | 115 | G |
| 1 | XA | 243 | A |
| 1 | XA | 244 | U |
| 1 | XA | 250 | A |
| 1 | XA | 266 | G |
| 1 | XA | 328 | C |
| 1 | XA | 345 | C |
| 1 | XA | 410 | G |
| 1 | XA | 412 | A |
| 1 | XA | 481 | G |
| 1 | XA | 484 | G |
| 1 | XA | 485 | G |
| 1 | XA | 509 | A |
| 1 | XA | 687 | A |
| 1 | XA | 703 | G |
| 1 | XA | 753 | A |
| 1 | XA | 812 | C |
| 1 | XA | 913 | A |
| 1 | XA | 991 | U |
| 1 | XA | 992 | U |
| 1 | XA | 1027 | C |
| 1 | XA | 1285 | A |
| 1 | XA | 1297 | C |
| 1 | XA | 1310 | G |
| 1 | XA | 1336 | C |
| 1 | XA | 1446 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | XA | 1498 | U |
| 23 | XX | 12 | A |
| 24 | YA | 99 | U |
| 24 | YA | 195 | A |
| 24 | YA | 221 | A |
| 24 | YA | 229 | A |
| 24 | YA | 242 | G |
| 24 | YA | 271(B) | G |
| 24 | YA | 278 | A |
| 24 | YA | 404 | C |
| 24 | YA | 503 | A |
| 24 | YA | 530 | G |
| 24 | YA | 637 | A |
| 24 | YA | 752 | A |
| 24 | YA | 846 | C |
| 24 | YA | 856 | C |
| 24 | YA | 859 | G |
| 24 | YA | 974(A) | C |
| 24 | YA | 1012 | U |
| 24 | YA | 1022 | G |
| 24 | YA | 1026 | U |
| 24 | YA | 1085 | A |
| 24 | YA | 1109 | C |
| 24 | YA | 1178 | C |
| 24 | YA | 1204 | A |
| 24 | YA | 1210 | A |
| 24 | YA | 1427 | A |
| 24 | YA | 1460 | A |
| 24 | YA | 1508 | A |
| 24 | YA | 1558 | A |
| 24 | YA | 1653 | G |
| 24 | YA | 1694 | C |
| 24 | YA | 1786 | A |
| 24 | YA | 1799 | G |
| 24 | YA | 1930 | G |
| 24 | YA | 1955 | U |
| 24 | YA | 1992 | G |
| 24 | YA | 2566 | A |
| 24 | YA | 2610 | C |
| 24 | YA | 2681 | C |
| 24 | YA | 2712 | U |
| 24 | YA | 2776 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 24 | YA | 2832 | U |
| 24 | YA | 2867 | G |
| 25 | YB | 66 | A |
| 22 | XV | 54 | G |

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1022 ligands modelled in this entry, 1020 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 56 | SF4 | XD | 301 | 4 | 0,12,12 | 0.00 | - | - | | |
| 56 | SF4 | QD | 301 | 4 | 0,12,12 | 0.00 | - | - | | |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 56 | SF4 | XD | 301 | 4 | - | - | 0/6/5/5 |
| 56 | SF4 | QD | 301 | 4 | - | - | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 56 | XD | 301 | SF4 | 3 | 0 |
| 56 | QD | 301 | SF4 | 1 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.